



Electrocatalysis and water treatment: Review

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Abstract

Electrocatalysis is a pivotal scientific discipline and a crucial part of industrial processes for the sustainable future for mankind. It is closely related to energy efficiency and the general processing rate of various electrochemical applications. Thus, a sound understanding of electrocatalysis provides versatile new functions and innovative solutions to numerous challenges we face in conventional and advanced technologies. Particularly, the challenges regarding the need for sustainable energy and water use arise with growing demands for more environmentally friendly, safer, and energy-efficient materials, which are less dependent on limited resources. In terms of resolving these challenging demands, the emergence of nanomaterials has brought a significant advance in technologies and enabled an in-depth and comprehensive understanding of electrocatalysis. In this review, we explore various electrochemical applications of both conventional and advanced technologies by categorizing them into five functioning groups: harvest, removal, consumption, storage, and analytics. For these applications with a particular aspect of sustainable energy and water, we discuss the roles and fundamentals of electrocatalysis, including technical parts such as cell configuration and its core elements, as well as the theories of thermodynamics and kinetics. Furthermore, we discuss how nanomaterials development and research activities have contributed to the deep understanding of nano electrocatalysis by reviewing some of the recent progress of various technologies. Finally, we explore the roles and the trend of these advanced nanomaterials in electrocatalysis with a focus on the properties and the design of materials.

Keywords: Electrocatalysis; Water Treatment; Pollutant Removal; Anodic Oxidation

1. Introduction

Over the years, rapid industrialization across the globe and other human activities have discharged a wide variety of chemicals into the water bodies and made them polluted. Ensuring a reliable and uncontaminated water source for both drinking and industrial use has grown increasingly difficult [1]. Electrocatalysis-based techniques are some of the promising technologies, which can be used in wastewater treatment. Electrocatalysts enhance the rate of electrochemical reactions taking place at the electrode surface or the solid/liquid interfaces [2]. In this review, different electrocatalysis techniques have been demonstrated for wastewater treatment applications. Further, it elucidates the fundamental ideas and mechanisms to comprehend electrochemical reduction/oxidation technologies and their application toward wastewater treatment.

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2. Types of catalyst

Catalysts can be classified in several ways. The main types are:

1. Positive catalyst

- Increases the rate of chemical reactions.
- Example: Iron (Fe) in the Haber process for ammonia production.

2. Negative catalyst (Inhibitor)

- Slows down the rate of chemical reaction.
- Example: Glycerol prevents the decomposition of hydrogen peroxide. [3]

3. Homogeneous catalyst

- Catalysts and reactants are in the **same phase** (all gases or all liquids).
- Example: Sulfuric acid (H_2SO_4) catalyzes the esterification reaction.

4. Heterogeneous catalyst

- Catalyst and reactants are in **different phases**.
- Example: Nickel (Ni) catalyzes the hydrogenation of vegetable oils.

5. Auto catalyst

- One of the products of the reaction acts as a catalyst.
- Example: Manganese ions (Mn^{2+}) formed during the reaction between potassium permanganate and oxalic acid.

6. Enzyme (Biocatalyst)

- Natural catalysts are produced by living organisms.
- Example: Amylase catalyzes the breakdown of starch into sugars [3,4].

Electrocatalysis uses applied electrical currents and specialized catalysts to drive chemical reactions that decompose water pollutants. It is highly effective for industrial wastewater, decomposing toxic organics and reducing contaminants like nitrates without requiring heavy chemical dosing or high-pressure operations

2.1. Why Electrocatalysis is Used

Traditional water treatment struggles with "forever chemicals" and toxic industrial runoff. Electrocatalysis solves this by offering unique advantages: [5]

- **No Chemical Sludge:** It uses electrons instead of bulk chemical additives.
- **Ambient Operations:** It runs efficiently at room temperature and normal pressure.
- **Targeted Destruction:** It completely breaks down tough toxins rather than just trapping them.
- **Renewable Power:** It can run directly on solar or wind electricity

The process takes place inside an electrochemical cell containing water, an anode (positive electrode), and a cathode (negative electrode).

Anode Reactions (Oxidation): The anode generates highly reactive oxygen species, like hydroxyl radicals ($\bullet\text{OH}$). These radicals attack and shred complex organic pollutants, such as pharmaceuticals, dyes, and pesticides, turning them into harmless carbon dioxide and water [6]

Cathode Reactions (Reduction): The cathode adds electrons to contaminants. This converts harmful, oxidized pollutants like nitrates (NO_3^-) into safe nitrogen gas (N_2), and plates out heavy metals (like lead or copper) into solid, recoverable forms [5,6]

3. Current Challenges

While highly effective in laboratory settings, widespread commercial use faces a few hurdles:

- **High Initial Cost:** Efficient electrodes often rely on expensive noble metals like platinum or ruthenium.
- **Catalyst Poisoning:** Impurities in real-world wastewater can coat the electrodes and lower their lifespan.
- **Energy Consumption:** Treating high volumes of highly diluted water can demand significant electricity.

Technology drives purification through several targeted mechanisms:

- **Electrocatalytic Oxidation:** Breaks down organic pollutants into benign byproducts (like CO_2 and H_2O) or more biodegradable compounds through direct charge transfer or the in-situ generation of strong oxidants like hydroxyl radicals.
- **Electrocatalytic Reduction:** Targets oxidized species such as nitrates and heavy metal ions, converting them into harmless nitrogen gas or solid deposits on the electrode surface.
- **Electro-Fenton Processes:** Uses electrical currents to continuously generate hydrogen peroxide (H_2O_2) and catalysts in the water, which together create powerful reactions to destroy recalcitrant organics.

Electrocatalysis provides a highly efficient, chemical-free method to destroy toxic water pollutants using electricity and advanced electrode materials. By driving chemical reactions directly on the surface of engineered catalysts, it breaks down complex toxins that traditional water filtration systems cannot remove. [7-11]

4. Core Processing Mechanisms

- **Anodic Oxidation:** Destroys organic pollutants (like pharmaceuticals, dyes, and pesticides) by generating highly reactive hydroxyl radicals ($\cdot\text{OH}$) on the positive electrode.
- **Cathodic Reduction:** Pulls electrons into inorganic pollutants on the negative electrode, transforming harmful nitrates into inert nitrogen gas and plating out toxic heavy metals.
- **Electro-Fenton Cycles:** Uses electrical currents to continuously generate hydrogen peroxide (H_2O_2) in-situ, maximizing the destruction of resilient "forever chemicals" like PFAS [12,13].

5. Key Operational Advantages

- **Zero Chemical Sludge:** Eliminates the need for bulk chemical dosing, drastically lowering secondary waste disposal costs.
- **Ambient Conditions:** Operates safely at room temperature and normal atmospheric pressure.
- **Green Energy Synergy:** Functions as a highly adaptive "plug-and-play" technology that can run directly on solar or wind power grids.
- **Decentralized Footprint:** Scales down easily into compact, automated units ideal for point-of-use industrial or rural treatment [14].

6. Current Implementation Barriers

- **Material Costs:** High-performance electrodes frequently require expensive noble metals (e.g., platinum, iridium).
- **Catalyst Fouling:** Real-world wastewater contains natural organic matter that can coat and deactivate electrode surfaces over time.
- **Mass Transfer Limits:** Shifting the technology from concentrated laboratory solutions to high-volume, highly diluted industrial wastewater requires complex reactor engineering [15].

7. Catalytic Techniques in Wastewater Treatment

7.1. Advanced Oxidation Processes (AOPs)

Photocatalysis is a light-activated catalytic process that uses semiconductor materials such as TiO_2 to generate reactive oxygen species (ROS). When irradiated with UV or visible light, electrons are excited from the valence band to the conduction band, forming electron-hole pairs. Advanced Oxidation Processes are treatment methods designed to generate hydroxyl radicals ($\bullet\text{OH}$), one of the strongest oxidants used in water treatment. These radicals react non-selectively with most organic contaminants (Figure 1).

Common AOPs : UV/ H_2O_2 / O_3 /UV Photocatalysis Fenton and Photo-Fenton Electrochemical oxidation

Pollutant Removal: Organic pollutants: Significant reduction in COD and TOC. Dyes: Cleavage of azo bonds and aromatic structures. Bacteria: Oxidative stress causes inactivation. Heavy metals: Oxidation state transformation enhances precipitation efficiency. pairs. These react with water and oxygen to produce hydroxyl radicals ($\bullet\text{OH}$) and superoxide radicals ($\text{O}_2\bullet^-$), which are highly oxidative [16,17].

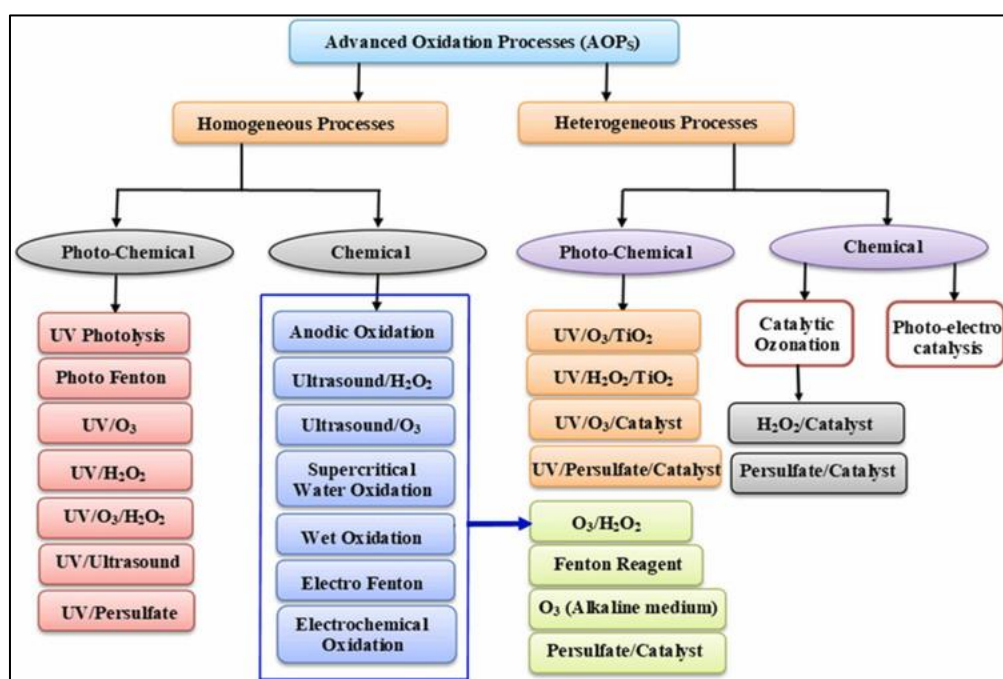


Figure 1 Classification of Advanced Oxidation Processes

7.2. Photocatalysis

Photocatalysis is a light-activated catalytic process that uses semiconductor materials such as TiO_2 to generate reactive oxygen species (ROS). When irradiated with UV or visible light, electrons are excited from the valence band to the conduction band, forming electron-hole pairs. These react with water and oxygen to produce hydroxyl radicals ($\bullet\text{OH}$) and superoxide radicals ($\text{O}_2\bullet^-$), which are highly oxidative.

7.3. Removal Mechanism

Organic pollutants: $\bullet\text{OH}$ radicals oxidize organic molecules, breaking aromatic rings and converting them into CO_2 and H_2O . **Dyes:** Chromophore groups are destroyed, leading to decolorization. **Bacteria:** ROS damage cell membranes and intracellular components. **Heavy metals:** Some metals such as Cr(VI) can be reduced to less toxic Cr(III) . Figure 2.Mechanism of photocatalytic degradation [18]

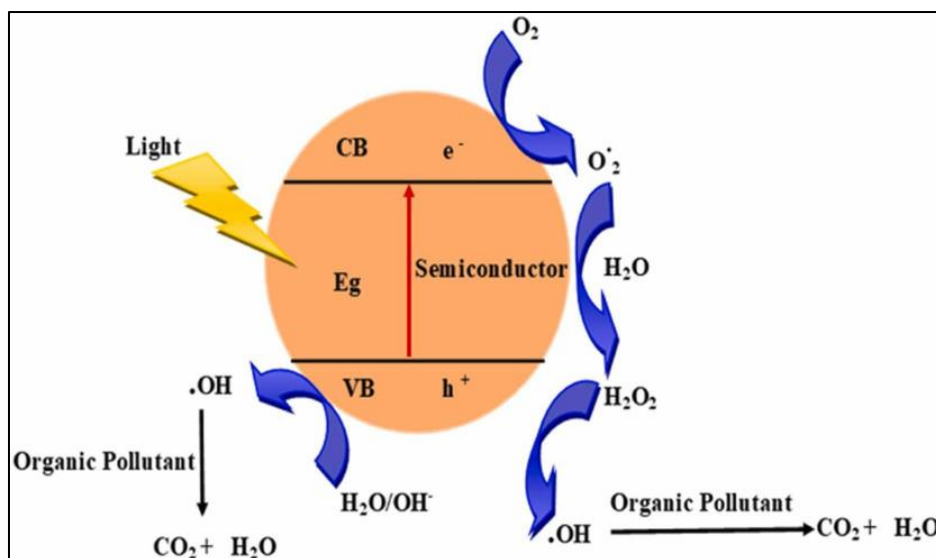


Figure 2 Photocatalytic mechanism showing electron–hole pair formation and ROS generation

7.4. Fenton and Photo-Fenton Reactions

The Fenton reaction involves the reaction of ferrous ions (Fe^{2+}) with hydrogen peroxide (H_2O_2) to generate hydroxyl radicals: $Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + \cdot OH + OH^-$. In the Photo-Fenton process, UV or solar irradiation enhances Fe^{3+} reduction back to Fe^{2+} , increasing radical production. Figure 3

Removal Mechanism:

- **Organic pollutants:** High degradation efficiency (>90% in optimized systems).
- **Dyes:** Rapid decolorization due to radical attack.
- **Bacteria:** Strong oxidative damage to cellular structures.
- **Heavy metals:** Enhanced removal when combined with coagulation or adsorption. Figure 3. [19,20]

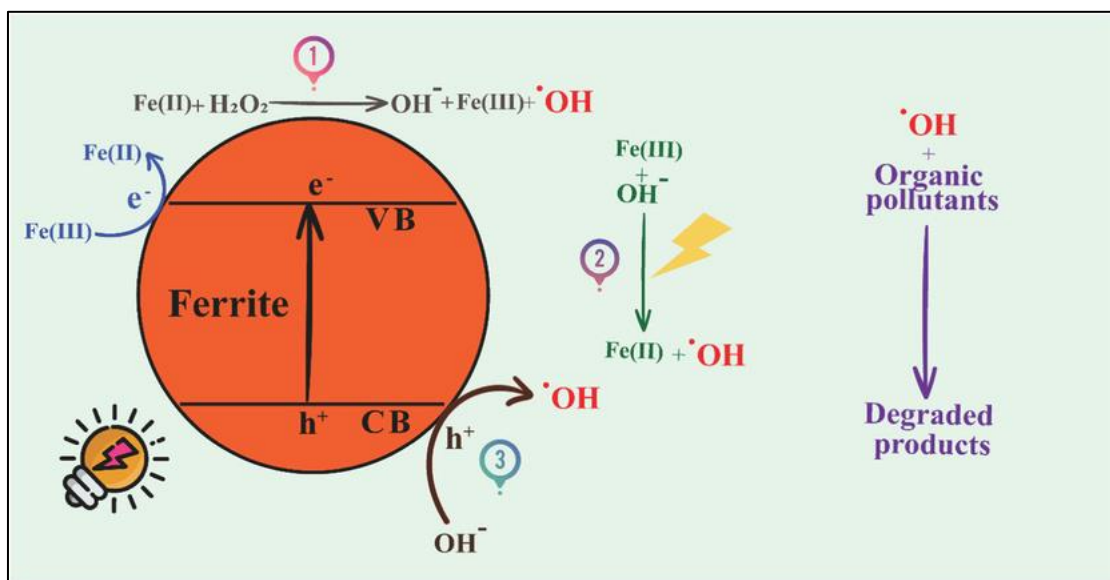


Figure 3 Reaction cycle of Fenton and Photo-Fenton processes

RuO_2 -Based Electrodes for Chlorine Evolution and Its Application in Water Treatment .Chlorine evolution now becomes important in many applications as chemical industry, polymer, pharmaceutical, and water treatment. In chlorine evolution reaction, the RuO_2 -based Dimensional Stable Anode is a technologically good and important electrode because of its unique characteristics such as high thermal and chemical stability, low resistivity, and low

overpotential. This reviews demonstrated the chlorine evolution reaction in the RuO₂-based electrode and its application in water treatment, especially in degradation of organic compounds and disinfection. The physicochemical, electrochemical properties and the mechanism of chlorine evolution at RuO₂-based electrode will be summarized in detail. Chlorine evolution reaction mainly happens at the electrode surface. Increasing chlorine evolution efficiency, stability and reducing energy consumption become critical issues for the sustainable development of chlorine evolution. The development of nanostructure material for chlorine evolution reaction is a hot topic for wastewater treatment soon [21].

A Novel Sol–Gel Synthesis Strategy of Co-Based Sillenite Composites for Enhanced Electrocatalysis of Water Splitting. This work reports a new synthetic strategy and investigates the effect of thermal treatment on Bi and Co oxide composites (BCO), comprising Co-based sillenite (Bi_{24–x}Co_x) Co₂O₄₀, Co₃O₄, and Bi₂O₃, as well as their application as electrocatalysts in the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). The materials were synthesized by a modified Pechini sol–gel method using citric acid as a complexing agent and ethylene glycol as a polymerization agent and were calcined in the range between 500 and 1000 °C. Rietveld refinement of the XRD data confirmed the predominance of the sillenite and Co₃O₄ crystalline phases, both with cubic structures, with minor quantities of α -Bi₂O₃ (monoclinic) at 500 and 600 °C. A higher sillenite content (>60 wt %) was observed at 700 and 800 °C, while at 900 °C the sillenite phase decreased, disappearing completely at 1000 °C, where α -Bi₂O₃ became dominant. The BCO sample calcined at 700 °C exhibited the lowest overpotentials for both the OER and HER in 1 mol L⁻¹ KOH (pH 14), 475 and 307 mV at j ± 10 mA cm⁻², respectively. The corresponding Tafel slopes for the OER and HER of 62 and 23 mV dec⁻¹, respectively, also exhibited the lowest values. The superior catalytic performance of BCO-T700 can be related to the synergy between Co²⁺ and Bi³⁺ species shown by X-ray photoelectron spectroscopy. These findings reinforce the potential of sillenite-based composites as efficient, low-cost, bifunctional electrocatalysts for water splitting and hydrogen production. Notably, no prior electrochemical studies of cobalt sillenites synthesized via the adapted Pechini method were found, emphasizing the relevance of this work [22].

Progress in Metal-Organic Framework Composites for Electrocatalytic Hydrogen Evolution Reaction. Metal-organic frameworks are extensively utilized in catalysis attributable to their huge porosities, even pore sizes and shapes, expandable pore surfaces, redox properties, and many other exceptional structural highlights that are easily tunable. In addition to the need for clean and maintainable technologies responsible for the storage and conversion processes of energy, together with the quick enhancement of the synthetic stability of these materials, metal-organic frameworks, and their composites are developing as unique electrocatalysts for the hydrogen evolution reaction. This investigation outlines demonstrative progress and highlights the significance of hydrogen evolution reaction and the structural property relationships of metal-organic frameworks. The metal-organic frameworks demonstrate the possibility to fill in as promising candidates for accomplishing high electrocatalytic exhibitions and studying electrocatalytic systems. More thought ought to be given to developing new metal-organic framework materials with high synthetic stability and electric conductivity and streamlining their crystal development on conducting substances for electrocatalytic hydrogen evolution reaction uses [23]

Copper-based electro-catalytic nitrate reduction to ammonia from water: Mechanism, preparation, and research directions. Global water bodies are increasingly imperiled by nitrate pollution, primarily originating from industrial waste, agricultural runoffs, and urban sewage. This escalating environmental crisis challenges traditional water treatment paradigms and necessitates innovative solutions. Electro-catalysis, especially utilizing copper-based catalysts, known for their efficiency, cost-effectiveness, and eco-friendliness, offer a promising avenue for the electro-catalytic reduction of nitrate to ammonia. In this review, we system antically consolidate current research on diverse copper-based catalysts, including pure Cu, Cu alloys, oxides, single-atom entities, and composites. Furthermore, we assess their catalytic performance, operational mechanisms, and future research directions to find effective, long-term solutions to water purification and ammonia synthesis. Electro-catalysis technology shows the potential in mitigating nitrate pollution and has strategic importance in sustainable environmental management. As to the application, challenges regarding complexity of the real water, the scale-up of the commercial catalysts, and the efficient collection of produced NH₃ still existed. Following research of catalysts, especially on long term stability and in situ mechanisms are proposed [24]

Photo electrocatalytic processes for the elimination of organic dyes from model aqueous systems .Dye industries produce large quantities of waste waters with visible colorization that cause non-esthetic pollution, serious health risks, and inhibit plant growth by impairing photosynthesis. Their bioaccumulation and recalcitrance can promote carcinogenicity, mutagenicity, and toxicity on aquatic beings and humans, requiring urgent decontamination. This article presents a comprehensive critical review of the development of photo electrocatalysis (PEC) applied to remediate organic dyes in synthetic aqueous solutions. Photogenerated electron/hole pairs at the photoanode by photocatalysis are produced under light irradiation (UV light, Visible light, and sunlight). These pairs produce oxidants

such as hydroxyl radical ($\bullet\text{OH}$) from H_2O_2 from O_2 oxidation with holes and reduction with electrons. The passage of electrons to the cathode prevents fast recombination of photogenerated carrier. Physiosorbed electrocatalysis from anodic H_2O_2 was also formed at the photoanode by O_2 oxidation. The preparation methods of novel photoanodes, the PEC systems used, the effect of operating variables that affect discoloration performance of dyes, the mechanisms that generate the oxidants, and reusability are detailed. Application of TiO_2 oxides, Bi compounds, $\text{g-C}_3\text{N}_4$, PbO_2 , ZnO , and WO_3 materials, Co and Fe, and other materials as photoanodes for organic dyes removal are described and analyzed. The performance of proposed hybrid PEC processes with O_3 , photoelectron-Fenton, sulfite, peroxy mono sulfate, and persulfate was finally discussed [25].

Role of Electrocatalysis in the Remediation of Water Pollutants. Providing a clean water supply for drinking or industrial use is challenging because of the variety of chemicals produced and used in daily life that end up contaminating water streams. 1 Agricultural and industrial processes create huge pollutant fluxes that inadvertently worsen water quality, with major offenders from global pesticide consumption (~ 3 million tons/year), 2 fertilizer usage (~ 200 million tons/year), 3 and synthetic organic chemicals production (>400 million tons/year). 4 The diversity and complexity of chemical water pollutants will require a range of treatment methods, including biological remediation, 5 physicochemical treatment, 6 and electrochemical methods such as electrochemical/electrocatalytic reduction, oxidation, and electrocoagulation. With the decreasing cost of renewable electricity and the increasing need to convert water pollutants to benign or useful chemicals, electrocatalytic treatment of polluted water is emerging as a viable remediation technology water treatment. 7 Electrocatalyst performance, however, is a major hindrance to the commercialization of these processes. In this Viewpoint, we discuss the role and feasibility of heterogeneous electrocatalysis for the treatment of water pollutants. We approach this problem from the lens of (electro)chemical engineering, which requires considering the role of the catalyst and reactor design, as well as overall process economics. Particularly, we analyze the effect of catalyst improvements in activity and selectivity on making the electrocatalytic treatment of wastewater practical. We focus our discussion on two case studies: namely, the electrocatalytic reduction of nitrate (NO_3^-) and the oxidation of phenol ($\text{C}_6\text{H}_5\text{OH}$). Nitrate reduction and phenol oxidation are chosen as examples because these pollutants are common, damage the environment, and are threats to human health. Separation methods are recognized to be key in addressing water pollution but are beyond the scope of this Viewpoint. The complexity of water pollutants presents two major obstacles for catalysis researchers working to combat water pollution: (1) how to identify if catalytic conversion of the target waste stream to the desired products is appropriate and competitive with alternative technologies and (2) how to understand the reaction mechanism and design better catalysts. While there has been significant effort on the second obstacle in literature, more consideration of the first obstacle is needed, in our opinion. Considerations of the type and scale of the target pollutant and the strengths and limitations of a potential electrocatalytic treatment method are emphasized here. We perform simple technoeconomic analyses to estimate the catalyst performance metrics needed to make water pollutant treatment feasible for nitrate reduction and phenol oxidation. Ultimately, in our view there are important, fundamental contributions to be made by both experimental and computational catalysis researchers in water pollutant remediation, but they should be guided by the practical challenges that would be encountered in commercial electrocatalytic reactors [26].

Advances and Prospects in Electrocatalytic Processes for Wastewater Treatment Wastewater pollution is severe, with various refractory compounds extensively used and discharged into sewage, posing risks to the environment and human health. Electrocatalytic technologies including direct and indirect electrocatalytic oxidation, electrocatalytic reduction, and electro-Fenton processes offer advantages such as high efficiency, ease of control, and minimal secondary pollution. This review aims to systematically introduce the principles, current research status, advantages, and disadvantages of various electrocatalytic processes used for wastewater treatment, with a focus on the electrode materials, operational parameters, and cost analysis of various electrocatalytic technologies. It also provides new insights into efficient electrode materials for future electrocatalytic technologies in treating refractory wastewater [27].

Activity and Selectivity Trends in Electrocatalytic Nitrate Reduction on Transition Metals. Electrocatalytic reduction is a promising approach to remediate nitrate (NO_3^-), one of the world's most widespread water pollutants. In the present work, we elucidate activity and selectivity trends of transition metals for electrocatalytic nitrate reduction to benign or value-added products such as N_2 and NH_3 . Using density functional theory (DFT) calculations, we find that the adsorption strengths of oxygen and nitrogen atoms act as descriptors for the overall activity and selectivity of nitrate reduction electrocatalysts. Nitrate reduction rates, volcano plots, surface species coverages, and the degree of rate control were predicted for transition metal electrocatalysts as a function of applied potential using DFT-based microkinetic modeling. Our microkinetic model rationalizes a few experimental observations including the activity trends of pure metals and our in situ X-ray absorption spectroscopy measurements of competitive adsorption between hydrogen and nitrate on Pt/C. We also predict that Fe_3Ru , Fe_3Ni , Fe_3Cu , and Pt_3Ru are promising catalysts for nitrate electroreduction toward N_2 with relatively high activity and selectivity. Ultimately, this work gives insight into nitrate

reduction on transition metal surfaces and can guide the design of improved electrocatalysts for nitrate remediation [28].

Water-Soluble Carbon Nano Onions-Augmented Microalgae for Coupled Wastewater Remediation and Biofuel Production: A Circular Economy Approach .The ever-increasing global energy crisis and wastewater burden demand a sustainable and integrated solution. A plausible solution that could address these issues is the utilization of wastewater as a raw material for biofuel production. Herein, the potential of waste cooking oil-derived water-soluble carbon nano onions (wsCNO) is explored in wastewater bioremediation and biofuel production. The microalgae *Chlorella pyrenoidosa* (*C. pyrenoidosa*) were cultivated in wastewater with different concentrations of wsCNO to assess the improvements in chemical oxygen demand (COD) abatement and lipid accumulation. *C. pyrenoidosa* treated with 20 mg L⁻¹ wsCNO achieved up to a ~56.16% higher COD abatement compared to the untreated control *C. pyrenoidosa*, while 1 mg L⁻¹ wsCNO led to a ~16.95% increase in the biomass yield. wsCNO efficiently reduced the COD without adversely affecting the lipid accumulation in microalgae. The present findings highlight the dual potential of wsCNO in promoting microalgal growth, photosynthesis, and bioremediation efficiency, which offers a futuristic circular economy approach for simultaneous wastewater treatment and renewable biofuel production [29].

MoS₂ Decorated 3D Graphene Aerogel as a Microwave Catalyst for the Ultrafast Breakdown of Organic Dyes .The effective, ultrafast, and complete removal of persistent and potentially toxic aromatic dyes continues to be a substantial challenge for the remediation of wastewater. Harnessing the unique adsorption capacity and catalytic activity of aerogels as microwave catalysts for the ultrafast degradation of organic contaminants in wastewater is on the rise. Herein, a MoS₂ decorated three-dimensional (3D) reduced graphene oxide aerogel (MoS₂-rGOA) that supported the ultrafast breakdown of methylene blue (MB) and crystal violet (CV) dyes under microwave irradiation is reported. The heterostructure of MoS₂-rGOA showed ultrafast and high microwave catalytic degradation of MB (97% in 8 min) and CV (94% in 10 min) dyes. The mechanistic features of the microwave catalytic dye degradation pathway assisted by MoS₂-rGOA, radical-trapping experiments, and optimized temperature, microwave power, and time are analyzed. Further, MoS₂-rGOA shows impressive efficacy in recycling and reuse, boasting both strong structural integrity and chemical stability. Its swift removal capabilities, ability to be recycled and reused, and cost-effectiveness showcase significant promise for widespread environmental cleanup in practical wastewater scenarios, a critical advancement in the field [30].

Transforming low-quality high-sulfur coal into porous heteroatom-doped carbon nano-onions for supercapacitor electrodes.Synthesizing low-cost carbon nanomaterials without relying on expensive raw materials, specialized equipment, or high energy input is crucial to meet the growing demand for affordable and eco-friendly solutions. In this study, high-sulfur low-quality coal is used as carbon source for the synthesis of porous heteroatom (N, S)-doped carbon nano-onions (h-CNOs) through a simple one-step thermal annealing process. Advanced structural and morphological analyses confirm the formation of multilayered, fused, concentric spherical graphitic structures in the h-CNOs, featuring high surface area and tunable porosity. The structural and compositional features enhance ion-diffusion, electrical conductivity, and surface wettability, making h-CNOs highly suitable for supercapacitors (SCs) applications. Further, the electrochemical evaluation of h-CNOs demonstrates the promising specific capacitance of 162 F g⁻¹ at a current density of 0.5 A g⁻¹ for supercapacitor application with stable capacity retention of 98% after 8000 cycles. The h-CNOs deliver a maximum energy density of 32 Wh kg⁻¹ and power density 24 kW kg⁻¹ in 6 M KOH aqueous electrolyte at a wide potential window of up to 1.2 V. Thus, this synthetic approach valorizes high-sulfur, low-quality coal feedstock by offering a scalable and efficient route for designing advanced carbon materials tailored for next-generation energy storage applications [31].

Simultaneous electrodeposition of multicomponent of Mn–Co–Ni oxides electrodes for phenol removal by anodic oxidation .Electrodeposition of metal oxides on graphite electrodes can improve their ability to remove organic substances. In this work, multicomponent oxides of Mn, Co, and Ni were electrochemically deposited on both the anode and cathode of graphite electrodes to enhance their performance in removing phenol. Formation of the deposit was achieved within 2 h in current densities of 20, 25, 30, and 35 mA/cm² for better composite properties. The deposited layer was characterized by testing the surface structure, morphology, composition, and roughness. X- ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX), and Atomic force microscopy (AFM) techniques facilitated these tests. The composite electrodes have synthesized with a metal salts concentration, i.e., Co(NO₃)₂, Ni(NO₃)₂, and MnCl₂ of 0.1 M with a mixing ratio of 1:1:1. The results exhibited a remarkable formation of the deposit on both the anode and cathode of our electrochemical cell. An amorphous skin of Mn–Co–Ni oxide was constituted on the anode, while a crystalline film of Mn–Co–Ni oxide accumulated on the cathode. The effectiveness of composite electrodes was examined at current densities of 40, 60, and 80 mA/cm², pH values of 3, 4 and 5, and NaCl concentration of 1, 1.5, and 2 g/l with an electrolysis time of 1 h. The results show that the removal efficiency of phenol increases with the increase in current densities and NaCl concentration, while it decreases with increasing of alkalinity.

The highest removal occurs at the pH, current density and NaCl concentration of 3, 80 mA/cm², and 2 g/l. The highest obtained removal efficiency is 99.68% which reflects a tremendously high performance of our multicomponent composite for phenol removal and reducing electrolysis time compared to previous studies [32].

Study of the kinetic model and the degradation process of the treatment of dye simulated wastewater using a coupled bio-electrochemical AF-BAF. **Experiments** were performed to investigate the mechanism of a biological anaerobic filter-biological aerobic filter (AF-BAF) process coupled with internal electrolysis for the treatment of dye simulated wastewater containing reactive brilliant red X-3B dye. A kinetic model of the anaerobic reactor was set up to provide the dependence of the COD removal rate on organic substrates (first-order) and the decolorization rate on dye concentration (first-order). Moreover, the results of gas chromatography/ mass spectrum (GC-MS) and UV-visible spectrophotometer (UV-Vis) analyses demonstrated that azo chromophore side groups were destroyed, and the degradation of benzene and naphthalene ring intermediates was intensified in the anaerobic stage by the coupled bio-electrochemical AF-BAF process. Additionally, the remaining benzene ring derivatives were further degraded by the subsequent aerobic stage [33].

Cadmium removal using a spiral-wound woven wire meshes packed bed rotating cylinder electrode. The effect of electrolysis operating parameters on the removal efficiency of cadmium from a simulated wastewater was studied by adopting response surface methodology combined with Box–Behnken Design. As a new electrode design, spiral-wound woven wire mesh rotating cylinder electrode was used for cadmium removal. Current (240–400 mA), rotation speed (200–1000 rpm), initial cadmium concentration (200–600ppm), and cathode mesh number (30–60) were chosen as independent variables while the removal efficiency of cadmium was considered as a response function. The results revealed that the rotation speed has the major effect on the removal efficiency of cadmium. Regression analysis showed good fit of the experimental data to the second order polynomial model with a coefficient of determination (R²) value of 0.9931 and Fisher F-value of 89.82. The optimal conditions within the experimental ranges of the independent variables were a current of 345 mA, a rotation speed of 800 rpm, an initial cadmium concentration of 500 ppm, and a mesh number of 30, where concentration of cadmium was diminished from 500 to 8 ppm after 60 min of electrolysis with a specific energy consumption of 3.12 kWh kg⁻¹ and a current efficiency of 41% [34].

Computational Catalysis and Machine Learning Applications to Water Treatment Technologies. **Electrocatalysis** can offer new routes to water treatment. For example, electrocatalytic reduction is an emerging technology for treating oxyanions of concern in water. However, identification of highly performant, cost-effective catalysts remains a major barrier to deployment at scale. This investigation discusses how computational modeling and machine learning can accelerate the search for new catalyst materials. It describes how traditional computational chemistry workflows, now deployed in their basic form for at least two decades, can be expanded in breadth and depth through newly developed machine-learned force fields that have been trained on millions of examples. It also discusses how the theory and machine learning pipeline can effectively integrate with experimental synthesis and characterization platforms to rapidly identify and validate new catalyst chemistries [35].

Carrier-driving CO₂ separation by amine-rich membranes with intercalated graphene oxide .Amine-rich facilitated transport membranes (FTMs) attract great interest in intensifying the membrane-based CO₂ separation processes. The high-molecular-weight polyvinylamine (PVAm) polymers containing fixed-site carriers of the amino groups were used to prepare highly CO₂-permeable membranes. The sterically hindered PVAm polymers of poly(N-methyl-N-vinylamine) and poly(N-isopropyl-N-vinylamine) were obtained by functionalization of PVAm to provide superior CO₂ solubility. By loading the mobile carriers of amino acid salt (AAS) and CO₂-philic graphene oxide (GO), the prepared FTMs render enhanced CO₂ permeance and CO₂/N₂ selectivity. The d-spacing of 8.8 Å and the ultra-micropores of 3.5 Å from GO nanosheets provide the combination of both selective surface flow and molecular sieving mechanisms to achieve improved CO₂ permeance and CO₂/N₂ selectivity. In addition, the intercalation of GO hinders N₂ transport through the membrane due to a longer pathway, while the mobile carriers of AAS introduced into the PVAm matrix facilitate CO₂ transport through the selective layer. Therefore, the CO₂/N₂ selectivity of the prepared FTMs was significantly enhanced to 171 based on the intensified carrier-driving transport mechanism. It can be concluded that amine-rich membranes based on both fixed and mobile carriers of the amino groups together with intercalated GO can synergistically improve the CO₂/N₂ separation performance and be potentially applied for CO₂ capture from flue gas [36].

Comparison of acid-resistant ceramic and polymeric nanofiltration membranes for acid mine waters treatment .Acid-resistant ceramic and polymeric nanofiltration (NF) membranes have been identified as relevant materials for sustainable management of acidic streams. NF properties such as a high passage of single-charged ions and high rejection of multi-charged ions make NF membranes suitable for acid recovery and metal concentration. In this work, the performance of two acid-resistant membranes: TiO₂ ceramic and MPF-34 (proprietary layer) was tested with

solutions mimicking acidic mine waters. Model solutions were composed by Al(III), Fe(III), Ca(II), Cu(II), Zn(II) and rare earth elements (REEs(III)) such as La(III), Dy(III), Sm(III), Nd(III), Pr(III) and Yb(III). The effect of acidity (from pH 1.5 to 1.0), Al(III) (from 0.6 to 1.8 g/L) and Fe(III) (from 0.5 to 2.1 g/L) concentrations was studied. Both membranes allowed the transport of H^+ (negative rejections were obtained), but exhibited differences related to the metallic ions transport. While MPF-34 presented metal rejections around 80% and independent on the concentration of the major components (Al(III) and Fe(III)), the TiO_2 membrane provided a sequence of rejection values from 5 to 30%, with highest values for trivalent transition metals. These differences in the sequence of rejections suggested that the chemical properties of the TiO_2 layer played a relevant role, and that they could only be explained by dielectric effects. From the observed rejections, it was estimated that MPF-34 provided concentration factors for metals up to 4.2 and <1 for the H_2SO_4 [37].

Nanocrystal-engineered thin CuO film photocatalyst for visible-light-driven photocatalytic degradation of organic pollutant in aqueous solution. We design a thin CuO film photocatalyst for visible-light-driven photocatalytic degradation of methylene blue (MB). Nanocrystal engineering of the photocatalyst is performed by sputtering with concurrent *in-situ* thermal treatment. The impacts of the *in-situ* thermal treatment temperature and sputtering conditions on the material properties of the thin CuO film photocatalyst are investigated in detail. Systematic characterization using field emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) indicates that deposition at elevated temperature and higher sputtering power significantly improves the surface structure and crystallinity of thin CuO film, which promotes charge transfer and ultimately results in better performance for MB photocatalytic degradation. The best-performing sample is the one sputtered at an elevated temperature of 300 °C and a sputtering power of 300 W. The photodegradation efficiency and physical durability of the samples were also analyzed after using for 5 cycles. The results indicate that *in-situ* thermal treatment and nanocrystal engineering of the thin CuO film significantly improve the physical durability [38].

Photocatalytic rate dependence on light absorption properties of different TiO_2 specimens. The light absorption and scattering play a prominent and often underrated role in the overall photocatalytic process and heavily affect the rate. This is particularly important for the choice of the catalyst in addition to other chemical and physical parameters usually considered for their catalytic role. Here we propose an approximate but easy-to-apply method to evaluate the light harvested by the photocatalyst slurry and its scattering/absorption coefficients, which does not require the use of complex spectrophotometric tools and the complicated radiative transport equation. The optical properties are obtained with the lamp and in the experimental setup employed in the photocatalytic batch tests. Among the four TiO_2 specimens considered, we characterized Evonik P25 and Hombikat UV100. The obtained scattering and absorption coefficients helped in rationalizing the experimental results on the degradation of formic acid at low concentration. From the rate dependence on the catalyst concentration, this approach allowed further understanding of the role of catalyst-specific properties affecting the overall catalytic performance. This approach is proposed as a starting point for fixing conditions to compare different photocatalysts [39].

Sensitizing effects of $BiVO_4$ and visible light induced production of highly reductive electrons in the $TiO_2/BiVO_4$ heterojunction. $BiVO_4$ is an efficient and stable visible active photoanode material. However, due to its unfavorable conduction band position which falls below the H_2 reduction potential, it fails to carry out the complete water splitting reaction. On the other hand, larger band gap TiO_2 can photo catalytically split water, thanks to its negative conduction band energy. Aiming at verifying the possibility of sensitizing TiO_2 with $BiVO_4$ and employing the so obtained composite material in photocatalytic water splitting under visible light, we prepared and photoelectrochemically characterized $TiO_2/BiVO_4$ heterojunction electrodes. The photocatalytic reduction of methyl viologen, an electron acceptor probe with a reduction potential close to that of protons, was used to evaluate the reducing ability of the photoactive materials under visible light. An apparently counterintuitive electron transfer from photoexcited $BiVO_4$ to the TiO_2 conduction band occurs in the $TiO_2/BiVO_4$ heterojunction, resulting in TiO_2 sensitization and production of highly reductive electrons, which appears to be favored by the band alignment occurring at the heterojunction [40].

Mn/Fe co-doped TiO_2 nanotube arrays for photoelectrochemical water splitting in neutral medium. Manganese and iron co-doped TiO_2 nanotube arrays (TNTs) are grown on Ti foil by in situ electro-anodization method and employed for overall photoelectrochemical water splitting. The band gap of TiO_2 is reduced from 3.3 eV to 3.1 eV with co-doping of Mn and Fe in Mn/Fe-TNT@Ti sample. Annealing Mn/Fe-TNT@Ti at 500 °C leads to the formation of trap states associated with the Fe^{3+} and Mn^{2+} ions present in the TiO_2 lattice. The anatase structure of TNTs in Mn/Fe-TNT@Ti-500 sample is confirmed by XRD and Raman spectroscopy. An anodic shift in the onset potential from 0.2 V_{RHE} to 0.08 V_{RHE} is observed in Mn/Fe-TNT@Ti-500 sample compared to Mn/Fe-TNT@Ti sample. The overall photocurrent density at $-0.4 V_{RHE}$ is higher for Mn/Fe-TNT@Ti-500 sample ($331 \mu A/cm^2$) than Mn/Fe-TNT@Ti sample ($251 \mu A/cm^2$). The oxygen evolution activity shows similar trend with Mn/Fe-TNT@Ti-500 displaying a photocurrent

density of $13.6 \mu\text{A}/\text{cm}^2$ at $1.23 V_{\text{RHE}}$. The anodic photocurrent density of Mn/Fe-TNT@Ti-500 sample is six times higher than that of the Mn/Fe-TNT@Ti at $0.8 V_{\text{RHE}}$. The incident photon to current efficiency (IPCE) measurements show that the photon absorption and conversion efficiency of the Mn/Fe-TNT@Ti-500 sample are significantly higher than that of the Mn/Fe-TNT@Ti sample. The results of this study complement the DFT calculations carried out with the generalized gradient approximation (GGA) technique. This work demonstrates possibility of designing composite materials for efficient photoreduction studies using n-type titanium nanotubes as precursors [41].

Advances in fuel cells EIS data analysis using the distribution function of relaxation times methods. Analyzing Electrochemical Impedance Spectroscopy (EIS) data measured on fuel cells is increasingly done by finding the Distribution Function of Relaxation Times (DFRT, also known as DRT). This has clear advantages in cases where the important loss mechanisms occur in series and at separable time constants. Then each peak may be attributed to a process, and its integral yields the effective loss associated with it [42].

Photocatalytic degradation of methylene blue dye by zinc oxide nanoparticles obtained from precipitation and sol-gel methods. Zinc oxide (ZnO) nanoparticles were synthesized by precipitation and sol-gel methods. The aim of this study was to understand how different synthetic methods can affect the photocatalytic activity of ZnO nanoparticles. As-synthesized ZnO nanoparticles were characterized by X-ray diffraction (XRD) and UV-Visible spectroscopic techniques. XRD patterns of ZnO powders synthesized by precipitation and sol-gel methods revealed their hexagonal wurtzite structure with crystallite sizes of 30 and 28 nm, respectively. Their photocatalytic activities were evaluated by photocatalytic degradation of methylene blue, a common water pollutant, under UV radiation. The effects of operational parameters such as photocatalyst load and initial concentration of the dye on photocatalytic degradation of methylene blue were investigated. While the degradation of dye decreased over the studied dye concentration range of 20 to 100 mg/L, an optimum photocatalyst load of 250 mg/L was needed to achieve dye degradation as high as 81 and 92.5% for ZnO prepared by precipitation and sol-gel methods, respectively. Assuming pseudo first-order reaction kinetics, this corresponded to rate constants of 8.4×10^{-3} and $12.4 \times 10^{-3} \text{ min}^{-1}$, respectively. Hence, sol-gel method is preferred over precipitation method to achieve higher photocatalytic activity of ZnO nanostructures. Photocatalytic activity is further augmented by better choice of capping ligand for colloidal stabilization, starch being more effective than polyethylene glycol (PEG) [43].

Highly efficient visible-light photocatalysis by Fe-substituted ZnO nanoparticles: Dual action on methylene blue degradation and microbial elimination. In this study Fe-substituted ZnO (Fe/ZnO) nanoparticles (NPs) are synthesized and utilized as an enhanced photocatalyst for the degradation of Methylene Blue (MB) and the inactivation of bacterial strains such as *S. aureus* and *E. coli*. The Fe/ZnO NPs were successfully synthesized using a sol-gel method assisted by combustion. Characterizations were performed using a range of analytical instruments, including Fourier Transform Infrared Spectroscopy (FTIR), X-ray Photoelectron Spectroscopy (XPS), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy with Energy Dispersive X-ray analysis (SEM-EDX), Brunauer–Emmett–Teller (BET) surface area analysis, Thermogravimetric Analysis (TGA), Photoluminescence (PL), and X-ray Diffraction (XRD). Compared to pure ZnO (24 nm) and other dopants, the resulting Fe(0.5 %)-ZnO nanohybrid exhibited a smaller particle size (12 nm). The degradation efficiency of the synthesized nanohybrids was evaluated by monitoring the degradation of Methylene Blue (MB) in an aqueous solution under visible light exposure. The photocatalytic efficiency of the synthesized Fe/ZnO nanohybrid was significantly higher within 120 min under consistent conditions, including pH:10, catalyst loading (50 mg), and MB dye concentration (10 ppm). Additionally, the antibacterial effectiveness of the samples was evaluated against two pathogenic strains (*S. aureus* and *E. coli*) using the agar diffusion method. At a concentration of 800 $\mu\text{g}/\text{mL}$, the Fe/ZnO nanohybrid demonstrated the highest inhibition (1.2 mm) of *S. aureus* growth, indicating that Fe doping enhances ZnO's antibacterial properties. The enhanced photocatalytic and antibacterial activities are attributed to the reduced band gap, increased visible light absorption, and improved charge separation caused by Fe doping, which leads to a greater generation of reactive oxygen species [44].

Microwave-assisted synthesis of ZnO nanoparticles using different capping agents and their photocatalytic application. This investigation reports the synthesis of ZnO nanoparticles from various sources of zinc salts via a microwave-assisted method. Furthermore, the synthesized ZnO nanoparticles were capped with different capping agents such as sodium hexametaphosphate (SHMP), polyvinylpyrrolidone (PVP), and cetylpyridinium chloride (CPC) to examine the stability and characteristics of ZnO nanoparticles. The synthesized ZnO nanoparticles were characterized with sophisticated analytical techniques such as XRD, FTIR, SEM, UV-vis DRS, Raman, and PL to understand their properties. From these studies, the XRD depicts the decrease in crystallinity of ZnO nanoparticles with the addition of different capping agents, and the morphology of the ZnO nanoparticles was influenced by capping agents as evidenced by SEM. The band gap of the synthesized ZnO nanoparticles is found to decrease with different capping agents confirmed by UV-Vis DRS studies. Furthermore, the photocatalytic degradation performance of the prepared samples is assessed by the degradation of methylene blue under visible light irradiation. The ZnO nanoparticles synthesized from the Zinc

nitrate source with SHMP capping agent show a greater extent of photocatalytic degradation efficiency than other Zinc sources. After 60 min of light, MB was observed to have degraded by about 80%, and hence, zinc nitrate is a suitable source to synthesize ZnO [45].

8. Conclusion

Electrocatalysis provides a highly effective, eco-friendly method for wastewater purification and remediation. It eliminates the need for harsh chemical additives by utilizing electrical currents to drive targeted redox reactions. This approach excels at breaking down persistent organic pollutants, deactivating bacteria, and safely removing heavy metals

Compliance with ethical standards

Disclosure of conflict of interest

I am interested in water treatment and removal of heavy metals using environmentally friendly materials also low-cost materials and applied electrochemistry like electropolishing, electroplating, and corrosion

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