

# Catalysts in Energy Applications

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## 1. Introduction

Catalysis stands as a fundamental driver in the energy landscape, influencing processes across the entire energy life cycle. From traditional fossil fuel production to emerging sustainable energy technologies like hydrogen fuel and artificial photosynthesis, catalytic processes play a pivotal role in shaping energy systems. This special issue delves into the intricacies of catalysis in energy applications, presenting research and reviews that highlight the nuanced relationship between catalytic processes and the evolving energy paradigm.

Traditional fossil fuel production relies heavily on catalytic processes to extract value from hydrocarbons [1-15]. Optimization of catalytic reactions in this context remains imperative for both efficiency and environmental considerations. As the energy landscape transitions towards sustainability, catalysis becomes instrumental in facilitating cleaner and more environmentally friendly alternatives, like biofuel production from renewable sources [9, 16-31] or CO<sub>2</sub> capture from the atmosphere, power plants or industrial facilities [32-39].

The shift towards sustainable energy introduces novel challenges and opportunities, and catalysis emerges as a key enabler in this transition. Hydrogen, as a clean energy carrier, represents a significant area of focus. Catalysis plays a critical role in hydrogen production, storage, and utilization, impacting the efficiency and viability of hydrogen as a sustainable energy vector [1, 19, 40-49].

In the pursuit of renewable energy, solar light-harvesting technologies have gained prominence. Catalysis takes center stage in these endeavors, particularly in the development of materials and processes for artificial photosynthesis. Mimicking nature's efficiency in capturing and converting solar energy into chemical energy, these advancements hold promise for sustainable energy generation [35, 37, 42, 44, 50-60].

The research papers presented in the Special Issue "Catalysts in Energy Applications" offer a detailed exploration of catalysis in diverse energy applications. From the synthesis of electrocatalysts for oxygen reduction reactions to theoretical insights into hydrogen evolution reactions, the contributions provide valuable insights into the intricate realm of chemical, electrochemical, and photochemical catalytic processes designed to address the challenges in energy-related domains.

## 2. Contributions

A significant portion of the research within this Special Issue is devoted to the Oxygen Reduction Reaction (ORR), a critical process in various energy conversion technologies [61-66]. Notably, the studies explored diverse non-precious metal catalysts, with a focus on advancing our understanding of ORR catalysts. Two manuscripts specifically investigated Perovskite-based catalysts, and others delved into coordination compounds-derived catalysts, primarily through pyrolysis or overoxidation processes.

Among the noteworthy contributions, the manuscript "MOF-Derived CuPt/NC Electrocatalyst for Oxygen Reduction Reaction" by Anwar et al. [67], introduces a novel

electrocatalyst synthesized through the pyrolysis of Cu-tpa MOF with low Pt loading, showcasing excellent ORR performance comparable to commercial Pt/C. The utilization of Metal-Organic Frameworks (MOFs) as precursors for nanocomposites is emphasized, highlighting their unique porous structures and stable electrochemical activity at higher temperatures.

Another significant theme in this Special Issue involves the use of Density Functional Theory (DFT) calculations to advance the understanding of ORR catalysis. The manuscript "Activating the FeS (001) Surface for CO<sub>2</sub> Adsorption and Reduction through the Formation of Sulfur Vacancies: A DFT-D3 Study" by Dzade et al. [68], presents a comprehensive investigation into CO<sub>2</sub> activation and reduction on defective FeS surfaces. Such mechanistic insights are invaluable in designing efficient catalysts for CO<sub>2</sub> conversion.

Furthermore, the manuscripts dedicated to Perovskite-based catalysts and coordination compounds-derived catalysts showcase innovative approaches in addressing the challenges associated with ORR. The study "Solid-State Ball-Milling of Co<sub>3</sub>O<sub>4</sub> Nano/Microspheres and Carbon Black Endorsed LaMnO<sub>3</sub> Perovskite Catalyst for Bifunctional Oxygen Electrocatalysis" by Karuppiah, et al. [69], introduces a highly efficient and durable LaMnO<sub>3</sub>@C-Co<sub>3</sub>O<sub>4</sub> composite, demonstrating excellent oxygen electrocatalysis in an alkaline environment.

Building upon the insightful contributions highlighted earlier, the Special Issue encompasses an array of other pioneering studies that extend the frontiers of catalysis for energy applications.

One such important article, "Enhanced Electrocatalytic Activity of Cobalt-Doped Ce<sub>0.8</sub>Er<sub>0.2</sub> Embedded on Nitrogen, Sulfur-Doped Reduced Graphene Oxide as an Electrocatalyst for Oxygen Reduction Reaction" by Sridharan et al. [70], introduces a synergistic electrocatalyst for the Oxygen Reduction Reaction (ORR). The combination of N- and S-doped reduced graphene oxide (rGO) with Co-doped CeO<sub>2</sub> demonstrated superior ORR performance in alkaline media. This study offers potential applications beyond traditional fuel cells and metal-air batteries, emphasizing the versatility of the synthesized electrocatalyst.

The manuscript "Inversion of the Photogalvanic Effect of Conductive Polymers by Porphyrin Dopants" by Petrov et al. [71] explores an intriguing inversion of the photogalvanic effect induced by doping NiSalen polymers with anionic porphyrins. This unexpected phenomenon, studied through UV-Vis spectroscopy and cyclic voltammetry, opens new avenues in understanding the interplay of conductive polymers and dopants, introducing a novel aspect in the realm of photoelectrochemical processes.

Furthermore, "Theoretical Insights into the Hydrogen Evolution Reaction on the Ni<sub>3</sub>N Electrocatalyst" by Cross et al. [72] provides a fundamental understanding of Ni<sub>3</sub>N surfaces for the Hydrogen Evolution Reaction (HER). Through dispersion-corrected density functional theory (DFT-D3), the study offers insights into the stability of Ni<sub>3</sub>N surfaces, water adsorption, and activation energies for HER. This comprehensive theoretical approach contributes valuable information for designing efficient Ni-based catalysts for HER.

The electrooxidation of urea, a crucial process for wastewater treatment, is addressed in the manuscript "Electrooxidation of Urea in Alkaline Solution Using Nickel Hydroxide Activated Carbon Paper Electrodeposited from DMSO Solution" by Aladeemy et al. [73]. The electrodeposition of nickel hydroxide on commercial carbon paper from dimethyl sulphoxide solvent resulted in a highly active and stable electrocatalyst for urea electrooxidation under alkaline conditions. This work introduces a promising approach for activating commercial carbon paper with transition metal electrocatalysts.

Additionally, "Benchmarking Perovskite Electrocatalysts' OER Activity as Candidate Materials for Industrial Alkaline Water Electrolysis" by Matienzo et al. [74] evaluates perovskite materials for the Oxygen Evolution Reaction (OER) in alkaline water electrolysis. The study considers industrial requirements and criteria, providing a systematic assessment of perovskite-based electrocatalysts for sustainable energy production.

The article "Bimetallic Cu/Pt Oxygen Reduction Reaction Catalyst for Fuel Cells Cathode Materials" by Alekseeva et al. [75] presents a bimetallic Cu/Pt catalyst prepared through a unique process, showcasing not only high activity in the ORR but also remarkable tolerance to the presence of methanol in solution. This work contributes to the ongoing efforts in designing efficient catalysts for fuel cell applications.

### 3. Conclusions

In conclusion, this Special Issue represents a significant stride in the field of catalysis for energy applications. The diverse range of catalysts explored, coupled with the application of advanced techniques such as DFT calculations, not only enhances our understanding but also opens avenues for the development of more efficient and sustainable energy conversion technologies.

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