6.1. Summary

In conclusion, this study systematically investigated the catalytic performance of mixed metal oxide systems, advancing from binary oxides to composite materials incorporating the conducting polymer polypyrrole. Initial evaluations focused on the base metal oxides, followed by strategic metal doping within the crystal lattice to enhance electrocatalytic activity. The results demonstrate that doping and polymer integration significantly improve catalytic performance and stability. These modifications not only optimize the electronic structure and active site availability but also highlight a viable approach for the rational design of high-performance electrocatalysts for future energy conversion applications.

In **Chapter 1**, the increasing global demand for clean and sustainable energy sources has been identified as a driving force behind the intensified research on electrochemical water splitting, with particular emphasis on the oxygen evolution reaction (OER), a critical half-reaction in hydrogen production. However, the sluggish kinetics of OER present a major bottleneck, necessitating the development of efficient electrocatalysts. Literature reveals substantial efforts in exploring various catalyst systems, including transition metal-based oxides, hydroxides, and their composites, to overcome this limitation. Mechanistic insights such as the Adsorbate Evolution Mechanism (AEM), Lattice Oxygen Mechanism (LOM), and Oxide Pathway Mechanism (OPM) have provided critical understanding of how intermediates evolve during OER in alkaline media. Each mechanism offers distinct pathways involving surface-adsorbed species, lattice oxygen participation, or metal–intermediate bond formation. These pathways have been instrumental in tailoring catalyst design for improved activity and durability. Metal doping, nanostructuring, and integration with conductive supports have further advanced the field. Overall, the literature underscores the importance of mechanistic understanding in driving the rational development of next-generation OER catalysts for scalable and efficient energy conversion systems.

In **Chapter 2,** various physicochemical and electrochemical techniques employed to comprehensively evaluate the OER catalyst's performance are discussed. FT-IR, Raman spectroscopy, XRD, FE-SEM, HR-TEM, BET, and XPS were used to study the structural, morphological, surface area, and compositional properties of the synthesized materials. Electrochemical analyses, including CV, LSV, EIS, and Tafel polarization curves, were carried out to assess the catalytic activity, stability, and kinetics. These techniques are essential for assessing important performance metrics that are essential for comprehending the stability and effectiveness of OER catalysts, such as the charge transfer resistance, Tafel slope, overpotential, and onset potential. These combined studies provided critical insights into the efficiency and durability of the catalysts. The integrated approach allowed for a systematic evaluation and optimization of materials for enhanced OER performance in alkaline media.

In **Chapter 3,** Mg-doped BCTO demonstrates promising potential as an OER electrocatalyst due to improved electrical conductivity, enhanced surface activity, and structural stability. The experimental findings showed that a semi-wet approach may be used to manufacture BCTO and Mg-doped BCTO in an easy and affordable way. The incorporation of Mg effectively modulates the electronic environment, leading to better charge transport and catalytic performance. An exceptionally small overpotential of 265 mV was recorded for $Mg_{0.1}$BCTO, with the lowest Tafel slope, the FTO/$Mg_{0.1}$BCTO electrode stood out as having the best electrocatalytic activity for OER in an alkaline environment among the tested BCTO and other Mg-doped BCTO variants. The effectiveness of this catalyst was highlighted by its virtually first-order kinetics for the OER reaction. These findings highlight Mg-doped BCTO as a viable candidate for future water-splitting applications.

In **Chapter 4,** the electrochemical performance of cobalt tungstate ($Co_xW_{2-x}O_4$; x = 0.5, 1.0, 1.5) catalysts in alkaline water oxidation was thoroughly examined. Our goal was to maximize long-term stability and catalytic activity by adjusting the cobalt-to-tungsten ratio. Among the various stoichiometries, the lowest overpotential was found to be 220 mV for $CoWO_4$ to provide 10 mA cm^{-2} current density. The composition with x = 1.0 performed the best overall, demonstrating an optimal balance of structural integrity, active site availability, and conductivity. Electrochemical studies revealed decreased overpotential, appealing Tafel slopes, and improved charge transfer kinetics. Morphological and surface studies confirmed stable interfaces and larger active surface areas. The results indicate that compositional adjustments are a helpful strategy for increasing OER activity. This work enables the development of durable and efficient mixed-metal oxide catalysts.

In **Chapter 5,** the $CoWO_4$/ppy composite exhibited excellent electrocatalytic activity toward OER in alkaline medium. The incorporation of ppy enhanced electrical conductivity, improved electron mobility, and increased exposure of active sites. The composite has shown a low overpotential of 350 mV at a current density of 10 mA cm^{-2} and exhibits a Tafel slope of 75 mV dec^{-1}. XRD, FT-IR, HR-TEM, XPS, and BET confirmed the well-defined structure and high surface area of the composite. Electrochemical studies showed low overpotential, favorable Tafel slope, and reduced charge transfer resistance. The material also demonstrated stable performance over prolonged operation, indicating good durability. The synergistic interaction between $CoWO_4$ and ppy played a crucial role in boosting overall catalytic efficiency. These results confirm the potential of $CoWO_4$/ppy as a high-performance, low-cost OER catalyst.

In conclusion, the comparative evaluation of Mg-doped BCTO, pristine $CoWO_4$, and $CoWO_4$/ppy underscores the superior electrocatalytic activity of the Co-based tungstate system. $Mg_{0.1}$BCTO required an overpotential of 265 mV to achieve 10 mA cm^{-2} with a Tafel slope of 92 mV dec^{-1}, whereas pristine $CoWO_4$ exhibited a ~17% reduction in overpotential (220 mV) and improved kinetics with a lower Tafel slope (75 mV dec^{-1}) and reduced charge-transfer resistance (56 Ω). Most notably, the $CoWO_4$/ppy composite achieved an exceptionally low overpotential of 170 mV at 10 mA cm^{-2}, representing a ~23% improvement compared to $CoWO_4$ and ~36% compared to Mg-doped BCTO, along with a significantly reduced Tafel slope of 61 mV dec^{-1}. These enhancements clearly demonstrate that the integration of conductive ppy with $CoWO_4$ not only optimizes charge transport but also maximizes the availability of catalytically active sites. Such substantial improvements highlight the uniqueness of Co-based tungstate/ppy composites as highly efficient and robust OER electrocatalysts, surpassing even the benchmark IrO_2.

6.2. Future Scope and Perspective

The catalysts discussed, including Mg-doped BCTO, $Co_xW_{2-x}O_4$, and $CoWO_4$/ppy composites, show significant promise for OER applications in alkaline media. Future work can focus on further tuning the composition, morphology, and surface chemistry to enhance intrinsic activity and durability. Advanced doping strategies, heterostructure formation, and interface engineering may unlock new reaction pathways and improve charge transfer. Moreover, integrating these catalysts into full electrolyzers systems and scaling up their synthesis will be critical for practical applications. Coupling experimental insights with theoretical modeling can also help in understanding the reaction mechanisms and guide rational catalyst design. Additionally, long-term operational studies under industrially relevant conditions are essential to validate the robustness and stability of these catalysts.

Furthermore, efforts should also focus on cost-effective and scalable synthesis methods, ensuring that these materials are both economically and environmentally viable for real-world applications. These future directions will play a pivotal role in advancing the development of next-generation electrocatalysts for green energy technologies.