ABSTRACT

The rapid development of efficient energy storage and conversion technologies is essential to mitigate the energy crisis and the environmental challenges associated with fossil fuels. Therefore, the development of effective electrocatalysts for energy conversion to produce valuable products is important for global sustainability. This study focuses on developing affordable and effective electrocatalysts for real-world applications. Here, I have specifically concentrated on the synthesis of bismuth-based electrocatalysts and their composites with carbon or hetero-atom-based carbon, such as Bi_2MoO_6, Bi_2MoO_6/carbon nanosheet, Bi_2MoO_6/g-C_3N_4, and $BiFeO_3$/g-C_3N_4, for various electrochemical applications. The Bi_2MoO_6 nanostructures were synthesized by a solvothermal approach by varying the solvent volume ratio and investigated as a low-cost electrocatalyst for nitrogen reduction reaction (NRR). The morphology significantly influenced the surface properties and, consequently, the electrocatalyst's activity, resulting in enhanced ammonia yield and faradaic efficiency. The oxygen reduction reaction (ORR) activity was studied using the same Bi_2MoO_6 electrocatalyst embedded with carbon nanosheets to improve the catalytic activity by increasing the surface area of the composite. The optimal composite with the highest concentration of oxygen vacancies was found to produce hydrogen peroxide via selective $2e^-$ ORR. The Bi_2MoO_6/g-C_3N_4 composites were also synthesized and examined for selective $2e^-$ ORR activity. The optimized electrocatalyst exhibits superior hydrogen peroxide selectivity and faradaic efficiency, owing to the highest electrochemically active surface area and the lowest charge-transfer resistance. To explore perovskite materials for effective $2e^-$ ORR application, $BiFeO_3$_ g-C_3N_4 composites were prepared. The highest concentration of oxygen vacancy defects identified in the optimized composite demonstrates good selectivity for the $2e^-$ ORR, resulting in a significant yield of hydrogen peroxide and high faradaic efficiency. To support the experimental findings and have a deeper understanding of the catalytic mechanisms, density functional theory (DFT) calculations were conducted. In summary, this dissertation significantly advances the field by developing cost-effective, efficient bismuth-based electrocatalysts that enhance electrochemical NRR and ORR activity to produce vital chemicals, such as ammonia and hydrogen peroxide, respectively.

Keywords: *Bi_2MoO_6, carbon nanosheet/Bi_2MoO_6, Bi_2MoO_6/g-C_3N_4, $BiFeO_3$/g-C_3N_4, NRR, ORR, ammonia, hydrogen peroxide, oxygen vacancy, yield, faradaic efficiency.*