Unveiling the ORR Mechanism on FePc: From Fundamentals to Practical Applications

Anuj Kumar
Department of Chemistry, GLA University, Mathura, UP-281406, India
Email: anuj.kumar@gla.ac.in (A. Kumar)

Abstract

The oxygen reduction reaction (ORR) is crucial for the efficiency of energy conversion devices, including fuel cells and metal-air batteries. Iron phthalocyanine (FePc) has emerged as a promising electrocatalyst due to its abundance, cost-effectiveness, and exceptional electrocatalytic activity. Understanding the core ORR process in FePc is crucial for optimizing its performance and moving from laboratory investigations to practical applications.

This talk will examine the mechanistic details of the ORR on FePc, focusing on its active sites, reaction routes, and kinetics using modern spectroscopic techniques and computational methods such as Density Functional Theory (DFT). Particular emphasis will be placed on the influence of central metal ions, axial ligand effects, and substrate interactions in regulating catalytic activity. Additionally, this talk will examine techniques to improve the ORR performance of FePc by structural alterations, heteroatom doping, and the creation of composite materials. The feasibility of FePc in practical applications will be assessed by its incorporation into fuel cell and battery systems. Comparative analyses with benchmark catalysts like Pt/C will demonstrate the viability of FePc as a sustainable alternative, facilitating its large-scale application in clean energy systems.

This talk aims to bridge the gap between fundamental science and practical deployment, offering a comprehensive perspective on the ORR mechanism and its implications for future energy systems.

Keywords: Iron phthalocyanine, electrocatalysts, ORR, DFT, clean energy, fuel cells.

References

1. Wang, W., Jia, Q., Mukerjee, S., & Chen, S. (2019). Recent insights into the oxygen-reduction electrocatalysis of Fe/N/C materials. ACS Catalysis, 9(11), 10126-10141.
2. Lopes, T., Kucernak, A., Malko, D., & Ticianelli, E. A. (2016). Mechanistic insights into the oxygen reduction reaction on metal–N–C electrocatalysts under fuel cell conditions. ChemElectroChem, 3(10), 1580-1590.
3. Kumar, A., Ibraheem, S., Nguyen, T. A., Gupta, R. K., Maiyalagan, T., & Yasin, G. (2021). Molecular-MN4 vs atomically dispersed M− N4− C electrocatalysts for oxygen reduction reaction. *Coordination Chemistry Reviews*, *446*, 214122.
4. Kumar, A., Vashistha, V. K., & Das, D. K. (2021). Recent development on metal phthalocyanines based materials for energy conversion and storage applications. *Coordination Chemistry Reviews*, *431*, 213678.