Engineering of Synergistic Fe-O Bonding in FePc-Graphene Oxide Quantum Dots Composite to Benchmark Oxygen Reduction Activity Beyond Pristine FePc

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Abstract

Iron phthalocyanine (FePc) nanostructures have been utilized to catalyse the slow kinetics of oxygen reduction reaction (ORR), an electrode process in fuel cells (FCs) and metal-air batteries (MABs), but their optimal performance has yet to be achieved. Herein, FePc-graphene oxide quantum dots (FePc-GOQDs) composite was synthesized using a hydrothermal-microwave approach and characterized by various techniques, revealing that the Fe–O bond formation between GOQDs and FePc altered FePc's electronic structure. The electrochemical tests showed that FePc-GOQDs composite had 300 mV, 100 mV, and 130 mV anodic shift in half-wave potential ($E_{1/2}$) with respect to GOQDs, 20% Pt/C, and pristine FePc due to Fe-O bonding. In addition, FePc-GOQDs had a low onset potential (+0.99 V), Tafel slop (40 mV dec^{-1}), methanol tolerance (negligible in $E_{1/2}$ after 5 mL methanol), and durability (negligible in $E_{1/2}$ after 10000 CV cycles), demonstrating excellent ORR performance. The theoretical results showed that Fe-O bonding optimised electronic properties (redistribution of charge density, density of states over the fermi level, HOMO-LUMO gap, and spin polarisation) of FePc-GOQDs, lowering the energy barrier of each ORR step compared to pristine FePc. Combining experimental and theoretical findings, this work provides a comprehensive understanding of ORR enhancement and mechanisms for FePc, assisted by external Fe-O bonding, enabling the development of future sustainable energy materials for FCs and MABs.

References

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