Effect of the surrounding carbon network for ORR activities of FeN4 embedded carbon catalysts for fuel cell

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Recently, nonprecious metal catalysts for oxygen reduction reaction (ORR) for fuel cells have drawn great attention as dispersed noble metal catalysts like platinum-based alloys have cost and durability issues. Carbon-based nonprecious transition metal catalysts proved to be cost-effective and electrocatalytically active with its superior current density and large surface area. In particular, carbon-based with FeN4 or FeN2 sites embedded in a sp2 hybridized carbon layer proved to have promising catalytic activity toward ORR. To extend understanding of the fundamental ORR mechanisms of the FeN4 embedded carbon layer, we investigate how the changes in carbon network around the active site are correlated with the ORR activities. To this end, we employ density functional theory (DFT) calculations and predict possible ORR pathways when the FeN4 site is embedded within a graphene layer with native defects. We investigate the energetics of both the dissociative and associative pathways for the FeN4 containing graphene layer with vacancy defects. Our DFT calculation results imply that the ORR activities can be modestly affected by the changes in the surrounding carbon network.