Mechanistic study of oxygen reduction reaction on functionalized $Fe/N_x/C$ catalysts

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Proton exchange membrane fuel cell (PEMFC) is an attractive energy conversion device due to its low operating temperature (<80ºC), fast start-ups, and low weight, etc. For this reason, it is expected to replace conventional power generators. However, the high price of Pt-based catalysts which are most widely used in PEMFCs is still main barrier to commercialize it. In this regard, non-precious metal catalysts (NPMCs) such as $M/N_x/C$ (M=transition metal) catalysts have been received a lot of attentions.
In this study, to improve the kinetic activity of Fe/Nx/C catalyst, we investigated the effect of electron withdrawing/donating properties of different types of sulfur functional groups in carbon plane on oxygen reduction reaction (ORR) activity by using density functional theory (DFT) calculations. On the basis of these results, we found that the change in ORR activity of the Fe-N-C catalysts would be originated from different electronic effects of different types of sulfur functional groups. Our results will be widely applied to design enhanced ORR catalysts for PEMFCs.