Theoretical study on pPy-assisted ORR of the metal-doped terephthalate

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Oxygen reduction reaction (ORR) is a cathodic reaction in fuel cell which is a promising candidate for clean energy conversion. To overcome the slow kinetics of ORR in the catalyst, a novel concept of involving polypyrrole (pPy) has been developed. The pPy is identified as co-catalyst to help catalysts to improve the kinetics in ORR. However, there have been only few theoretical studies on how pPy accelerates the ORR. Therefore, by using density functional theory calculations, the effect of pPy on the ORR was investigated with metal-doped terephthalate system in this study. We used GGA+U method for 3d-transition metal ions to localize d-orbitals, which is usually calculated to be delocalized with conventional GGA method. We found that the secondary amine of pPy was deprotonated during ORR to accelerate the reaction and recovered at the end. The deprotonation of pPy usually occurred at the reaction $*O \rightarrow *OH$. We also found that some catalysts were hardly affected by pPy because they strongly interacted with deprotonated pPy, making the recovering step of the pPy difficult. Through this study, we firstly suggested that the deprotonation of pPy induced the enhanced efficiency of ORR.