Design and Strategy of Nitrogen Doped Graphene for the Enhanced H_2O_2 Selectivity during Oxygen Reduction Reaction and Water Oxidation Reaction

박성오, 임형용, 이경민, 곽상규†
울산과학기술원
(skkwak@unist.ac.kr†)

Due to the increase of H_2O_2 demands in various fields such as paper bleaching, chemical synthesis, and waste water treatment, much effort has been devoted for developing the efficient methods for H_2O_2 production. Electrochemical H_2O_2 production method has been suggested as an eco-friendly alternative. However, it heavily relies on the electrode so that the electrodes for the efficient electrochemical H_2O_2 production should be found or newly designed. Thus, we investigated that the nitrogen doped graphene with topological defects to propose the design of the carbon materials towards the highly selective and efficient electrochemical H_2O_2 production. We first determined the stability of the nitrogen doping on topological defects as well as that on the hexagonal lattice. Subsequently, the relationship between the structural stability and the efficiency of H_2O_2 production was predicted with the results of H_2O_2 reaction mechanism. Through this relation, a strategy for nitrogen doping on graphene was theoretically proposed towards high electrochemical performance of H_2O_2 production.