Electrochemical water splitting on graphene surface activated by mono-and di-vacancies by DFT calculation

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When graphene is exposed to ion/electron irradiation, vacancy defects, which activate the graphene surface, were easily formed. In this theoretical study, we showed defective graphene could be used as good electrochemical catalyst for water splitting reaction. First, vacancy site on defective graphene was investigated by electron/spin density and orbital analysis. Electrons were localized on dangling carbon atoms, which became active sites for the reaction. On mono-vacancy defect, oxygen molecule was strongly adsorbed. On the other hand, dangling carbon atoms on di-vacancy defect could form pentagonal ring (i.e. 5-8-5 defect) with neighboring carbon atoms. This hexagon-pentagon transition facilitated the graphene surface to produce oxygen molecule as a product of water splitting. By estimating the Gibbs free energy of intermediate structure of water splitting reaction (e.g. OH*, O*, and OOH*), we demonstrated that, indeed, di-vacancy defects made the graphene surface a possibly good catalyst for the oxygen evolution reaction using water.