Density Functional Theory Study on the Catalytic Behavior of OH Functionalized N-Doped Graphene for Oxygen Reduction Reaction in Fuel Cells

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Abstract

Catalytic behavior of metal-free Hydroxyl group (OH) functionalized single nitrogen (N-Gra(OH)16), and triple nitrogen (N3-Gra(OH)16) doped graphene surface are investigated in the 4e- reduction pathway under oxygen reduction reaction (ORR) process. The thermodynamical parameters indicate the reaction to be highly exothermic and feasible with the N-Gra(OH)16 and N3-Gra(OH)16 as catalysts. However, N3-Gra(OH)16 shows better catalytic properties than N-Gra(OH)16. First, all reactive species (*O2, *OOH, *O, and *OH) chemisorb via a covalent bond on the N3-Gra(OH)16, which is essential for the efficient reaction kinetics. Secondly, the product H2O is physisorbed on the N3-Gra(OH)16, required for the uninterrupted reaction cycle. Categorically, the N3-Gra(OH)16 shows excellent catalytic activity due to a higher number of nitrogen atoms which has a lowered EHOMO-LUMO gap, concomitantly increasing the surface's reactivity. Besides the above, the barrier energies are comparable with platinum (Pt) catalyst. Our results show that the N3-Gra(OH)16 surface is the most suitable catalyst for ORR activity.

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