DFT Study of P-Doped Bilayer Graphene Configuration on the ORR in Acidic Solution

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ABSTRACT

Fuel cells, particularly polymer electrolyte membrane fuel cells (PEMFCs), generate electricity and water through chemical reactions, using air pollution as fuel, making them a leading technology for the green economy. The oxygen reduction reaction (ORR) at the catalyst layer significantly influences the cost and electrochemical performance of fuel cells. Recently, non-platinum group metals (non-PGMs) have emerged as promising catalysts for their low cost and high catalytic performance in PEMFCs. This study examines the electronic properties and electrocatalytic activity of single P-doped monovacancy (PC3-BLG) and divacancy (PC4-BLG) of AB bilayer graphene in sulfuric acid membrane solutions. The results demonstrate that PC3-BLG exhibits greater stability and superior electrocatalytic activity compared to PC4-BLG. PC3-BLG is predicted to have an indirect energy gap of approximately 0.46 eV, indicating a transition from half-metallic to small bandgap semiconductor properties, while PC4-BLG suggests a *p*-type semiconductor. An activation energy of 0.54 eV was found in PC3-BLG, with the rate-limiting step being the second H_2O formation, positioning it as a promising alternative non-PGM catalyst to Pt/C in acidic solutions. These findings offer potential strategies for using carbon-based materials in designing efficient non-PGM catalysts for ORR.

Reference

[1] Pham, N.N.T.; Nguyen, V.K.T.; Guo, H.; Lee, S.G. Influence of phosphorus-doped bilayer graphene configuration on the oxygen reduction reaction in acidic solution. *Carbon* **2023**, *210*, 118012.