Density Functional Theory Study of Sensing Mechanism of Gas Molecules on Defective Graphene for High-Sensitivity Gas Sensor

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Graphene has huge potential as a gas sensor due to the high carrier mobility, large specific surface area, and low electrical noise. It is reported that defective graphene showed the enhanced response to gas molecules. However, the mechanism governing the sensing of gas molecules in defective graphene remains unclear. To elucidate the sensing mechanism of graphene as a function of the type of defects, density functional theory (DFT) calculations were performed by investigating the optimized geometries and the corresponding charge transfers upon the adsorption of gas molecules. Our results indicated that vacancy defects are the main contributors to the gas sensing performance. We also examined the vacancy formation energy of graphene adsorbed on gold nanoparticle. Our approach will provide useful insight into the promising materials for gas sensor based on graphene.