A DFT Study for Selective Gas Sensing on Functionalized Graphene

정관영, 이태경, 차진혁[1], 곽상규[†]

울산과학기술원; [1]현대모터스

(skkwak@unist.ac.kr[†])

Graphene has been accepted as a promising material for chemical gas sensor because of its superior electrical, mechanical and thermal properties. However, a low binding affinity to target gases in its pristine state has hampered practical applications. In order to overcome this obstacle, graphene functionalization can be a suitable approach to enhance the chemical sensitivity. We have chosen NH_3 and NO_2 molecules, which are common toxic gases while exhibiting the contrasting charge transfer characteristics of electron-donating (i.e., NH_3) and electron-withdrawing (i.e., NO_2) behaviors. Using these as target gases, we investigated the interaction mechanisms of the gases on the functionalized graphene by density functional theory calculations. We initially examined the feasibility of functionalization of various functional groups by formation energy calculations. Subsequently, the most plausible candidates of functional groups for each target gas were systematically found by comparing the binding energy and charge transfer amounts. This study provides a fundamental understanding about interaction mechanisms that can govern the selective detection of toxic gases.