ABSTRACT

Volatile organic gas such as formaldehyde, acetaldehyde, and acetone is carcinogenic chemical group which leads increasing cancer risk such as leukemia in long term exposure. Previous study has shown 9 times more increasing adsorption value of formaldehyde on heterostructures graphene-boron nitride (G/h-BN) compared to reduced graphene oxide. So, we will be focus to discover deeper based on previous result through computational study to get advanced understanding of adsorption at quantum level. In order to manifest this study, DFT (Density Functional Theory) method was used to optimize and calculate intermolecular interaction. In solid state modelling, few parameters such as cutoff energy, k-point, exchange correlation functional, and dispersion function were optimized first. Then, those three ligands of formaldehyde, acetaldehyde, and acetone along with both receptors graphene and G/h-BN were optimized before interacting each other. We put every ligand of formaldehyde, acetaldehyde, and acetone in 12 different orientations above graphene and G/h-BN receptor to find the most optimal adsorption orientation. The result showed cutoff energy was converged at 680 eV, k-point grid size in 7x7x1 and 15x15x1, PBE as GGA exchange correlation functional, and vdW-DF2 as the most relevant dispersion functional based on previous study. The complex system optimization of ligand and receptor showed increasing adsorption strength on G/h-BN receptor compared to graphene receptor through increasing adsorption energy value. It is found that adsorption energy has increased about 0,864 kJ/mol in formaldehyde adsorption, 3,08 kJ/mol in acetaldehyde adsorption, and 3,682 kJ/mol in acetone adsorption. The orientation of each system showed similar pattern which carbonyl group sits over hollow of graphene and sits over carbon atom of G/h-BN.

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Keywords*: Volatile organic gas, hetero graphene boron nitride, solid state, DFT, Quantum ESPRESSO*