Ab Initio Calculations on the Adsorption of Cadmium and Lead on Graphene and Graphene Oxide

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Adsorption of Cadmium (Cd) and Lead (Pb) was studied on graphene (Gr) and graphene oxide (GO) using first principle density functional theory (DFT). The electronic and structural properties of these heavy metals on periodic supercells were investigated using the hybrid generalized gradient approximation (GGA) functional PBE0 implemented in CRYSTAL14 software. Gaussian basis sets of 6-311G(d) for C and O and 3-1G(p) for H atoms were used. For Cd and Pb, effective core potential (ECP) basis sets were implemented. Three adsorption sites on Gr and GO were investigated –namely hollow (H), top (T) and bridge (B) sites. The binding energies and equilibrium distances for the most favorable adsorption sites on Gr were calculated and compared for different coverages of Gr supercells ranging from 2×2 to 6×6. The optimized structures showed that H site was the most energetically preferable site for Cd adsorption; while for Pb, T site was the most favorable one.[1] Compared to Cd, the adsorption energy for Pb with Gr was higher by about 0.66 eV. For GO, three different structures with the most stable coverages were studied: epoxy, hydroxyl and epoxy-hydroxyl groups as shown in Figure 1.[2] According to the results, there was an enhancement in the binding energy for some sites over others with respect to pure Gr. For instance, Pb adsorption energy at the B site of epoxy graphene was more stable by ~0.41 eV than that of pure Gr. However, when Pb was positioned above the oxygen atom, the calculated adsorption energy was low, compared to other sites on Gr. These results indicated that the presence of oxygen-containing functional groups strengthens the adsorption of these heavy metals in specific positions. The band gap and density of states diagrams were also analyzed to understand the interaction of the heavy metals with GO. Based on our study, GO can be an excellent material for water treatment applications.

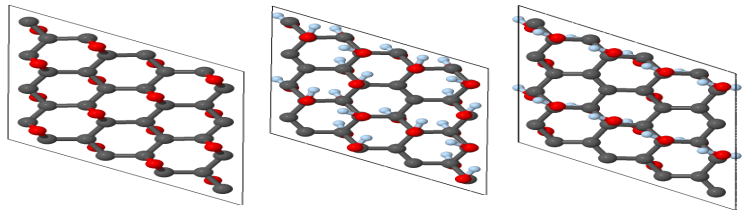

Fig. 1. the optimized structures of epoxy, hydroxyl and epoxy-hydroxyl graphene (from left to right) and the coverages are 100%, 75%, and 75%, respectively.

1. K. Nakada, and A. Ishii, *Solid State Commun.* **2011**, 151, 13-16.
2. D. W. Boukhvalov, and M. I. Katsnelson, *JACS*. **2008**, 130, 10697-10701.