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제일원리기법을 이용하여 Graphene에 분산된 Li 금속 원자의 수소 흡착 특성 및 안정성에 대한 연구

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Developing efficient and stable hydrogen storage media is very crucial for hydrogen economy. One of the most promising materials suggested as a potential hydrogen storage media is a carbon based material such as carbon nanotube, fullerene and graphene. Recently, metal adsorbed graphene shows very good results which satisfy the target of DOS 2010 system. However, contrary to theoretical result, some experimental study presented poor results of graphene because of reducing surface area by an agglomeration of graphene sheet. Moreover, it is well known that the maintenance of open metal state is very hard, since the dispersed metal atom on graphene can absorb non-hydrogen atoms such as carbon, oxygen and nitrogen. Therefore, the detail study about metal dispersed graphene is needed inevitably in order to find high capacity hydrogen storage material. In this study, the hydrogen adsorption properties of Li dispersed graphene with boron substitution were investigated by using ab intio method.

The total energy calculations and the structural relaxations were performed by using a plane wave based density functional theory (DFT) with the Vienna ab initio simulation package (VASP) The graphene system is represented in a supercell by a slab of one graphene sheet and a vacuum region of 16 Å. Graphene sheet is composed of 4/4 carbon/boron atoms and 16/16 carbon/boron atoms for the (2 × 2) and (4 × 4) graphene sheet, respectively. It is found that Li atoms are well dispersed on boron substituted graphene and can form the (2 × 2) pattern. Clustering of Li atoms is hindered by repulsive Coulomb interaction between Li atoms. Li adatom dispersed on the double side of graphene can absorb up to six hydrogen molecules and hydrogen storage capacity can be increased to 11.40%. Moreover, adsorption behaviors of non-hydrogen atoms such as C, B, and O2 are calculated to know whether Li atom can continue open metal state in boron substituted graphene.