PENGARUH LOGAM Li PADA ADSORPSI ATOM-ATOM H OLEH PERMUKAAN GRAFENA PLANAR

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ABSTRACT

Graphene has future prospect for electronics. By adding some substituents this material can be tuned to behave like a metal or semiconductor. In this investigation, a planar single layer of modified graphene, $C_{24}H_{12-m}Li_m$ (m = 0, 3, 6, and 12) consisted of seven six-member rings was used to adsorb the oncoming hydrogen (perpendicular to the surface, was defined as H_{ad}). A planar twolayer graphene $C_{48}H_{24}$ (7+7) was also included. To determine the adsorption models and the H_{ad} couverage, a semiempiris Calzaferri program, works on pentium 4 windows 98, was used to optimize nH_{ad} (n = 1, 2, and 3) that reached the surfaces. The heat of H_{ad} adsorption and the band gap of the surfaces were also computed. Results of these computations showed that: (1) the adsorption process was endothermic and Li reduced the heat of H_{ad} adsorption on the surfaces. (2) Li reduced the band gap of the surfaces, so $C_{24}H_{12}$ was a semiconductor but $C_{24}Li_{12}$ a conductor. (3) The adsorbed nH_{ad} always lowered the band gap of the surfaces, in exception of $C_{24}Li_{12}$ could be lower or higher. (4) Each atom on the surfaces, in exception hydrogen, might adsorb nH_{ad} formed tilted (with C) and lying down (with Li) surface complexes, and for $C_{24}H_6Li_6$ an asymmetric twofold complex was also observed. (5) However, the H_{ad} couverage was low, some H_{ad} formed H_2 and this was not observed on $C_{24}H_6Li_6$. (6) The $C_{48}H_{24}$ kept an H_2 molecule between layers. Thus, a new material $C_{24}H_6Li_6$ which had two adsorption models, might increase the H_{ad} couverage, but had lower conductivity than that of $C_{24}H_{12}$. On the other hand, it is necessary to study in more details the hydrogen storage between graphene layers.

***Key words**: graphene, adsorption, substituent*

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 ISSN : 1978-628X