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} coverage, a semiempiris Calzaferri program, works on pentium 4 windows 98, was used to optimize n_{H_{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 n_{H_{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 n_{H_{ad}} formed tilted (with C) and lying down (with Li) surface complexes, and for C_{24}H_{3}Li_{6} an asymmetric twofold complex was also observed. (5) However, the H_{ad} coverage was low, some H_{ad} formed H_{2} and this was not observed on C_{24}H_{3}Li_{6}. (6) The C_{48}H_{24} kept an H_{2} molecule between layers. Thus, a new material C_{24}H_{3}Li_{6} which had two adsorption models, might increase the H_{ad} coverage, 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

DAFTAR PUSTAKA

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