INTISARI

Adsorpsi Hidrogen pada Monovacancy h-BN: Kajian Komputasi Menggunakan DFT (*Density Functional Theory*)

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Adsorpsi hidrogen dan air pada *monolayer* hexagonal boron nitride (h-BN) telah dipelajari dengan menggunakan teori fungsi kerapatan (DFT). Dua konfigurasi *monovacancy* dimodelkan, yaitu *monovacancy* nitrogen (V_N) dan *monovacancy* boron (V_B) dengan menghilangkan atom N dan B dari lembaran h-BN. Supercell yang terdiri dari 32 atom digunakan untuk menganalisis adsorpsi hidrogen dan air (H2O) dengan menghitung energi formasi dan adsorpsi. Dari perhitungan energi adsorpsi negatif, ditemukan bahwa reaksi yang terlibat bersifat eksotermik, artinya hidrogen dan air mudah teradsorpsi pada lembar h-BN. Selain itu, sistem hidrogen di lokasi V_B merupakan sistem yang paling stabil yang ditunjukkan dengan energi formasi terendah sebesar 2,78 eV.

Kata-kata kunci : h-BN, monovacancy, energi adsorpsi dan formasi, penyimpanan hidrogen.

ABSTRACT

Hydrogen Adsorption on Monovacancy h-BN: Computational Study Using DFT (The Density Functional Theory)

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Hydrogen and water adsorption on the monolayer hexagonal boron nitride (h-BN) has been studied using the density functional theory (DFT). Two configurations of monovacancy were modeled, which are monovacancy at nitrogen site (V_N) and monovacancy at boron site (V_B) by removing N and B atoms from the h-BN sheet, respectively. A supercell consisting of 32 atoms was used to analyze the adsorption of hydrogen and water (H2O) by calculating formation and adsorption energies. From the calculated negative adsorption energies, we found that the involved reactions are exotermic, meaning that hydrogen and water are easily adsorbed on the h-BN sheet. In addition, a system of hydrogen at V_B site was the most stable system shown by the lowest formation energy of 2.78 eV.

Keywords : h-BN, monovacancy, adsorption and formation energies, hydrogen storage.