ABSTRAK

Penelitian ini mengonstruksi grafik hubungan antara *surface coverage* dan energi adsorpsi atom Oksigen (adsorbat) di atas permukaan Pt (adsorben). Ada lima variasi *surface coverage* yang digunakan, yaitu 0,25 ML; 0,50 ML; 0,75 ML; dan 1,00 ML. Selain variasi *surface coverage*, adsorpsi atom Oksigen dirancang terjadi pada tiga posisi berbeda, yaitu: *top, hollow* dan *bridge*. Kalkulasi proses adsorpsi dilakukan berbasis *density functional theory* (DFT). Kalkulasi DFT memberikan nilai energi total elektronik sistem yang digunakan untuk menghitung energi adsorpsi, yang kemudian diplot pada grafik bersama nilai *surface coverage* untuk mendapatkan korelasi keduanya. Plot tersebut menunjukkan bahwa perubahan nilai *surface coverage* memengaruhi nilai energi adsorpsi. Penelitian ini berhasil mengonstruksi grafik hubungan antara energi adsorpsi dan *surface coverage*. Ada dua posisi setelah hasil optimisasi yaitu posisi *hollow* dan *top*. Posisi *hollow* menghasilkan hubungan kuadaratik jika titik satu adsorbat dihilangkan sedangkan posisi *top* menghasilkan hubungan $[-\exp(-x)]$. Permukaan yang stabil memiliki energi adsorpsi yang negatif. Adsorpsi oksigen dengan *surface coverage* 0,75 ML dengan dua belas adsorbat pada posisi *hollow* menghasilkan energi paling negatif yaitu -6,860 eV. Sehingga sistem yang stabil adalah 0,75 ML pada posisi *hollow*.

Kata kunci: Adsorpsi, *Surface Coverage*, *Density Functional Theory*.

ABSTRACT

This research construct the plot of adsorption energy of oxygen atom (adsorbate) at Pt surface (adsorbent) as a function of surface coverage. There are five variation of surface coverage used in this research: 0.25 ML; 0.50 ML; 0.75 ML; and 1.00 ML. The adsorption of oxygen atom was designed to happen on three different position: top, hollow, and bridge. Calculation of adsorption process was done based on Density Functional Theory (DFT). DFT calculations give total electronic energy of the system. This energy then used to calculate the adsorption energy. The plot between the adsorption energy and surface coverage shows that the surface coverage have correlation with the adsorption energy. The DFT optimization gives two stable position of oxygen atom– hollow and top. Hollow position shows quadratic plot while top position gives $[-\exp(-x)]$ plot. The stable surface have negative adsorption energy. Adsorption of 12 oxygen on hollow position at surface coverage 0.75 ML gives the most negative energy: -6.860 eV. This shows that the most stable system is the hollow at 0.75 ML surface coverage.

Keywords: Density Functional Theory, adsorption, surface coverage.