

ABSTRAK

Simulasi kuantum reaksi pemisahan karboksil (COOH) pada permukaan PtMo(111) berbasis *density functional theory* telah dilakukan. Penelitian ini dilakukan untuk mencari tahu kemungkinan terjadinya reaksi pemisahan COOH_(ads) menjadi CO_{2(ads)} dan H_(ads), serta untuk memahami mekanisme pemisahan reaksinya pada permukaan PtMo(111). Hal yang dilakukan untuk mencapai tujuan tersebut yaitu mensimulasikan situs-situs adsorpsi COOH_(ads) dan koadsorpsi CO_{2(ads)} + H_(ads) pada permukaan PtMo(111) menggunakan metode *density functional theory* (DFT). Kemungkinan terjadinya reaksi pemisahan COOH diketahui melalui energi aktivasi. Energi aktivasi diperoleh dengan metode NEB. Metode NEB merupakan metode dengan konsep mencari lintasan dengan energi minimum untuk menemukan keadaan transisinya. Hasil dari penelitian ini adalah reaksi pemisahan COOH_(ads) menjadi CO_{2(ads)} dan H_(ads) pada permukaan PtMo(111) sangat mungkin terjadi dengan energi aktivasi sebesar 0,26 eV. Reaksi pemisahan tersebut terjadi karena gugus COOH_(ads) yang telah terbentuk teradsorpsi di situs *top* Pt sehingga memecah menjadi CO_{2(ads)} dan H_(ads), dengan CO_{2(ads)} di situs *bridge* PtMo dan H_(ads) di situs *top* Pt. Muatan elektron di sekitar molekul CO_{2(ads)} diketahui berpindah menuju atom Pt dan Mo, sedangkan muatan atom H_(ads) diketahui berpindah menuju atom Pt di permukaan. Hal tersebutlah yang memicu gugus COOH_(ads) memisah menjadi CO_{2(ads)} dan H_(ads). Jika ditinjau dari LDOS yang diperoleh, interaksi CO_{2(ads)} dan H_(ads) di situs tersebut sangat kuat dan stabil. Hal tersebut ditunjukkan oleh intensitas *peak* di daerah anti-*bonding* yang rendah dan adanya hibridisasi orbital dengan permukaan, serta *peak* di daerah *bonding* yang keberadaannya energinya sangat minimum.

Kata kunci : DFT, PtMo(111), adsorpsi, koadsorpsi, NEB.

ABSTRACT

A quantum simulation of the carboxyl separation (COOH) reaction on the surface of $\text{PtMo}(111)$ based on density functional theory has been carried out. This research was conducted to find out the possibility of $\text{COOH}_{(\text{ads})}$ separation into $\text{CO}_{2(\text{ads})}$ and $\text{H}_{(\text{ads})}$, and to understand the mechanism of the reaction separation on the PtMo surface (111). What was done to achieve this goal was to simulate $\text{COOH}_{(\text{ads})}$ adsorption sites and $\text{CO}_{2(\text{ads})}$ adsorption + $\text{H}_{(\text{ads})}$ on the surface of $\text{PtMo}(111)$ using the density functional theory (DFT) method. The possibility of $\text{COOH}_{(\text{ads})}$ separation reaction is known through activation energy. Activation energy is obtained by the NEB method. NEB method is a method with the concept of finding a path with minimum energy to find the transition state. The results of this study are the reaction of the separation of $\text{COOH}_{(\text{ads})}$ to $\text{CO}_{2(\text{ads})}$ and $\text{H}_{(\text{ads})}$ on the surface of $\text{PtMo}(111)$ is very likely to occur with an activation energy of 0.26 eV. The separation reaction occurs because the $\text{COOH}_{(\text{ads})}$ group that has formed is adsorbed at the top Pt site so that it breaks down into $\text{CO}_{2(\text{ads})}$ and $\text{H}_{(\text{ads})}$, with $\text{CO}_{2(\text{ads})}$ at the PtMo and $\text{H}_{(\text{ads})}$ bridge sites at the Pt top site. The charge of electrons around the $\text{CO}_{2(\text{ads})}$ molecule is known to move towards the Pt and Mo atoms, while the charge of the $\text{H}_{(\text{ads})}$ atom is known to move towards the Pt atom on the surface. This is what triggers the $\text{COOH}_{(\text{ads})}$ group to separate into $\text{CO}_{2(\text{ads})}$ and $\text{H}_{(\text{ads})}$. When viewed from the LDOS obtained, the interaction of $\text{CO}_{2(\text{ads})}$ and $\text{H}_{(\text{ads})}$ on the site is very strong and stable. This is indicated by the intensity of the peak in the anti-bonding area is low and the hybridization of the orbitals with the surface, and the peak in the bonding area where the presence of energy is very minimum.

Keywords: DFT, $\text{PtMo}(111)$, adsorption, adsorption, NEB.