ABSTRAK

Penggunaan sumber energi berbahan bakar fosil yang masih mendominasi di berbagai sektor tidak hanya membuat persediaan bahan bakar fosil di alam semakin berkurang, tetapi juga memberikan dampak yang tidak baik bagi lingkungan. Permasalahan ini membuat penelitian mengenai sumber energi alternatif seperti *Direct Methanol Fuel Cell* (DMFC) terus dilakukan baik secara eksperimen maupun teoritis. Simulasi kuantum berbasis metode *density functional theory* (DFT) untuk interaksi gugus *formate* dengan permukaan Pt(111) telah dilakukan. Penelitian ini mengkaji salah satu reaksi *intermediate* dari sel bahan bakar metanol di bagian anoda yaitu interaksi gugus *formate* ($HCOO^-$) dengan katalis Pt. Studi tentang simulasi kuantum ini bertujuan untuk menentukan konfigurasi interaksi dan mekanisme adsorpsi $HCOO^-$ dengan permukaan Pt(111). Mekanisme interaksi antara adsorbat dan permukaan dibahas dengan analisis transfer muatan. Penelitian telah berhasil menentukan situs paling stabil dari interaksi antara $HCOO^-$ dengan Pt, yaitu konfigurasi *side-on* berupa dua atom O teradsorpsi ke permukaan. Selanjutnya, dari analisis beda rapat muatan dan analisis bader ditemukan bahwa interaksi terjadi melalui transfer muatan dari permukaan ke adsorbat. Lebih jauh lagi, dari analisis *Density of State* diperoleh kesimpulan bahwa interaksi didominasi oleh orbital p_z pada atom O. Selanjutnya, ikatan atomik terbentuk dari pemakaian bersama elektron yang ditandai pelepasan elektron dari atom Pt dan penambahan elektron pada atom O.

Kata kunci : *Direct Methanol Fuel Cell*, Adsorpsi, *Density Functional Theory*, Gugus *Formate*, $HCOO^-$, Pt(111).

ABSTRACT

The use of fossil fuel-based energy sources which still dominates in various sectors not only reduces the supply of fossil fuel in nature, but also has negative impact on the environment. This problem makes research on alternative energy sources such as Direct Methanol Fuel Cell (DMFC) has been performed both experimentally and theoretically. Quantum simulation for interaction of formate on Pt(111) was performed using density functional theory method. This research studied one of the intermediate reaction of the direct methanol fuel cells at the anode, especially the interaction of the formate ($HCOO^-$) with Pt catalyst. This quantum simulation studies aim to determine the interaction configuration and adsorption mechanism of $HCOO^-$ on Pt(111) surface. The mechanism interaction of adsorbat and surface was explained by using charge transfer analysis. Research has succeeded in determining the most stable site interaction between $HCOO^-$ and Pt, that was side-on configuration which two O atoms adsorped onto the surface. Furthemore, from the charge density difference analysis and bader analysis, it was found that the interaction occurred through charge transfer from surface to adsorbate. In addition, from the Density of State analysis it can be concluded that the interaction was dominated by p_z orbital on O atom. Furthemore, atomic bonds was formed from sharing electrons which was marked by the loss of electrons from Pt atom and the addition of electrons to the O atom.

***Keywords** : Direct Methanol Fuel Cell, Adsorption, Density Functional Theory, Formate, $HCOO^-$, Pt(111).*