O-2

Magnetism during adsorption of oxygen in Pt segregated Pt_3Ni (111): Density Functional Study

Sharma Bharat Kumar*, Kwon Oryong, Dorj Odkhuu, Hong Soon Cheol
Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, 680-749, Ulsan, Republic of Korea
Tel: +82-(0)52-259-2331 Fax. +82-(0)52-259-1693

ABSTRACT

Limited understanding of the surface properties of Pt_3Ni for the oxygen reduction reaction (ORR) in polymer electrolyte membrane fuel cell (PEMFC) has motivated the study of magnetic properties and electronic structures of Pt segregated Pt_3Ni (111) surface during adsorption of oxygen molecule on it. The first principle method based on density functional theory (DFT) is carried out. Nonmagnetic Pt has induced magnetic moment due to strong hybridization between Ni 3d and Pt 5d. It is found that an oxygen molecule prefers bridge site with Pt rich subsurface environment for adsorption on the surface of Pt segregated Pt_3Ni (111). It is seen that there is very small charge transfer from O_2 to Pt. The curve of energy versus magnetic moment of the oxygen explains the magnetic moments in transition states. We found the dissociation barrier of 1.07eV significantly higher than dissociation barrier 0.77eV on Pt (111) suggesting that the dissociation is more difficult on Pt segregated Pt_3Ni (111) surface. The spin polarized densities of states are presented in order to understand electronic structures of Pt and O_2 during the adsorption in detail.

Keywords: Fuel cell, Pt_3Ni, density functional theory, magnetic properties, electronic structure