Magnetic Properties and Electronic Structure of Pt_3Ni (001), (110) and (111) Surfaces: Density Functional Study

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ABSTRACT

The 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 properties and electronic structures of seven layered Pt_3Ni (001), (110), and (111) surfaces. The first principle method based on density functional theory (DFT) is carried out. It is found that the bulk Pt_3Ni has a ferromagnetic ground state with the ordered fcc type L12 structure, which is in good agreement with other results. Non magnetic Pt has the induced magnetic moment due to the strong hybridization between 3d Ni and 5d Pt. The magnetic moment of Pt and Ni enhanced on the surface of each due to surface effect however the magnetic moment of surface Pt in the Pt–segregated Pt3Ni (111) decreased and the magnetic moment of Ni in Ni rich subsurface increased significantly. The calculated d band centers of Pt explain the possibilities for oxygen absorption and play the important roles in altering the catalytic properties. The spin polarized densities of states are presented in order to understand physical properties of Pt in different surfaces in detail.

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