World Academy of Science, Engineering and Technology
International Journal of Chemical and Molecular Engineering
Vol:12, No:01, 2018

Modeling of Anode Catalyst against CO in Fuel Cell Using Material Informatics

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Abstract : The catalytic properties of metal usually change by intermixturing with another metal in polymer electrolyte fuel cells. Pt-Ru alloy is one of the much-talked used alloy to enhance the CO oxidation. In this work, we have investigated the CO coverage on the Pt2Ru3 nanoparticle with different atomic conformation of Pt and Ru using a combination of material informatics with computational chemistry. Density functional theory (DFT) calculations used to describe the adsorption strength of CO and H with different conformation of Pt Ru ratio in the Pt2Ru3 slab surface. Then through the Monte Carlo (MC) simulations we examined the segregation behaviour of Pt as a function of surface atom ratio, subsurface atom ratio, particle size of the Pt2Ru3 nanoparticle. We have constructed a regression equation so as to reproduce the results of DFT only from the structural descriptors. Descriptors were selected for the regression equation; xa-b indicates the number of bonds between targeted atom a and neighboring atom b in the same layer (a,b = Pt or Ru). Terms of xa-H2 and xa-CO represent the number of atoms a binding H2 and CO molecules, respectively. xa-S is the number of atom a on the surface. xa-b- is the number of bonds between atom a and neighboring atom b located outside the layer. The surface segregation in the alloying nanoparticles is influenced by their component elements, composition, crystal lattice, shape, size, nature of the adsorbents and its pressure, temperature etc. Simulations were performed on different size (2.0 nm, 3.0 nm) of nanoparticle that were mixing of Pt and Ru atoms in different conformation considering of temperature range 333K. In addition to the Pt2Ru3 alloy we also considered pure Pt and Ru nanoparticle to make comparison of surface coverage by adsorbates (H2, CO). Hence, we assumed the pure and Pt-Ru alloy nanoparticles have an fcc crystal structures as well as a cubo-octahedron shape, which is bounded by (111) and (100) facets. Simulations were performed up to 50 million MC steps. From the results of MC, in the presence of gases (H2, CO), the surfaces are occupied by the gas molecules. In the equilibrium structure the coverage of H and CO as a function of the nature of surface atoms. In the initial structure, the Pt/Ru ratios on the surfaces for different cluster sizes were in range of 0.50 - 0.95. MC simulation was employed when the partial pressure of H2 (PH2) and CO (PCO) were 70 kPa and 100-500 ppm, respectively. The Pt/Ru ratios decrease as the increase in the CO concentration, without little exception only for small nanoparticle. The adsorption strength of CO on the Ru site is higher than the Pt site that would be one of the reason for decreasing the Pt/Ru ratio on the surface. Therefore, our study identifies that controlling the nanoparticle size, composition, conformation of alloying atoms, concentration and chemical potential of adsorbates have impact on the steadiness of nanoparticle alloys which ultimately and also overall catalytic performance during the operations.

Keywords : anode catalysts, fuel cells, material informatics, Monte Carlo
Conference Title : ICTCC 2018 : International Conference on Theoretical and Computational Chemistry
Conference Location : Zurich, Switzerland
Conference Dates : January 15-16, 2018