

Catalytic activity of core-shell nano-cluster based on platinum for hydrogen oxidation reaction: all-electron DFT study

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In a fuel cell device such as proton exchange membrane (PEMFC), the catalytic activities on each electrode play a pivotal role in determining a whole performance. Platinum has been widely used since it exhibits excellent catalytic activity in this device, however, there is a serious hindrance due to high cost and small reserves for commercialization. It is needed to discover a novel catalyst that has lower cost and stronger activity than that of platinum catalyst. For this purpose, recently, many researches have been done for the binary alloys composed of core-shell structure based on platinum by using various transition metals. We have studied the catalytic activity of Pt-based alloy for the hydrogen oxidation reaction on anode for application in PEMFC. As an alloying element, we considered Ag, Au and Cu and assumed these elements acted as a core material. We compared the adsorption energy between these core-shell nano-clusters and the pure Pt nanoparticle and investigated a chemical trend among these metals. The details will be presented in later.