Functional Nanoparticle Simulations of Catalysis for Fuel Cell

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Abstract

Nanoparticle, which means a fine particle in nanometer scale, is promising material for several industrial applications. Nanoparticle consisting of transition metals seems to be good electrode catalysis. In order to develop a new stable and high-performance Pt-based catalysis, it is an urgent problem to understand the reduction of catalysis poisoning by carbon monoxide (CO). In previous works using the Earth Simulator, we provided a possible of the reduction of CO-poisoning, which several transition metal elements add into Pt-based catalysis. In this work, we examine the relation between the reduction of CO-poisoning and the surface modification of Pt-catalysis.

The electronic structure calculation was carried out based on density functional theory with PBE96 formulation for the exchange-correlation energy functional. The simulation uses a model system, which consists of five-layered Pt(111) slab under the three-dimensional periodic boundary condition. And, we constructed a point defect surface in Pt(111) slab by removing a Pt-atom from the surface of Pt(111)-p(4x2) slab. The CO molecule, oxygen atom and CO_2 molecule connect Pt(111)-surface. The atomic positions of point-defect surface and reactants (CO, O) were determined by the first-principles molecular dynamics methods. Actual performance of the present version of PHASE (Ver. 7.01) showed 0.25 TFLOPS using 16 nodes of the Earth Simulator.

In this work using the Earth Simulator, We obtained the following results of understanding a reduction of the CO poisoning:

1. The adsorption energies of oxygen atom, CO molecule and CO2 molecule increase nearby the point-defect on Pt-surface.
2. Oxygen atom adsorb on an edge-site of the point-defect, a reduction of the reaction barrier of CO oxidation is obtained on which the oxygen atom participates in the CO oxidation.
3. Oxygen atom adsorb on a 3-fold hollow site of nearby point-defect, reduction of the reaction barrier of CO oxidation is NOT obtained on which the oxygen atom participates in the CO oxidation.

Keyword: Nanoparticle, Fuel Cell, Platinum-based catalysis, Defect, CO poisoning, First-principles density functional theory calculation