Functional Nanoparticle Simulations of Catalysis for Fuel Cell

Project Representative

Takashi Yoshida

Toshiba Corporation, Corporate Research and Development Center

Authors

Takashi Yoshida[*1], Yasutaka Nishida[*1], Satoshi Ito[*1], Hiroya Suno[*2]

＊1　Toshiba Corporation, Corporate Research and Development Center

＊2　Japan Agency for Marine-Earth Science and Technology

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 for Fuel Cell (FC). Conventionally, electrode catalysis for FC consists of platinum and platinum-based alloys containing several transition metals. In order to develop a new stable and high-performance catalysis of FC-electrode, it is an urgent problem to understand the chemical reaction of methanol decomposition and the reduction of anode poisoning by carbon monoxide (CO). We focused on the electric structures and CO oxidation reaction energy profiles on the platinum-based alloy surface. 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 three-layered Pt(111) slab under three-dimensional periodic boundary condition. The CO molecule and oxygen atom connect Pt(111)-surface. The atomic positions of alloy and ligands (CO, O) were determined by the first-principles molecular dynamics methods. Actual performance of the present version of PHASE (Ver. 6.01) showed 0.24 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 CO poisoning:

- The CO oxidation reaction is significantly accelerated on the composition ratio of "Pt:Ru = 3:1", while the CO oxidation reaction is suppressed on ruthenium-enriched surface, That is, the composition ratio in surface layer of Pt/Ru catalyst correlates with the activity of CO oxidation reaction.

It is expected that these theoretical results give a clue to develop a new functional catalysis in industrial development phase.

Keyword: Nanoparticle, Fuel Cell, Catalysis, Platinum-based alloy, CO poisoning, the First-principles density functional theory calculation