Search for Advanced Functional Materials concern with Eco-products

Project Representative

Takashi Yoshida

TOSHIBA Corporation Corporate Research and Development Center

Takashi Yoshida[*1], Fumihiko Aiga[*1], Misako Iwasawa[*2]

＊1　TOSHIBA Corporation, Corporate Research and Development Center

＊2　Japan Agency for Marine-Earth Science and Technology

Abstract

Graphenes have mono atomic-layer and honeycomb lattice of carbon materials in which it looks like a structure of physical peeling from graphite. It is a candidate for next generations of electronic devices, such as sensors, conductive films, catalysts and so on. For applications of these devices, we have interests in the feature of electronic structures of the graphenes. In this particular project, we focus upon the disability of hydrogen evolution reactions (HER) under the conditions of the Oxygen reduction reaction (ORR) on the graphene materials. Additionally, we explained its unique affections for nitrogen substitutions.

In this work using the Earth Simulator, we unreached a good understanding of the disability of HER on edged-graphene with nitrogen substitutions. However, we obtain some characteristic results for proton affinity of armchair-edge and zigzag-edge graphene with nitrogen compared with a case of oxygen molecule adsorption at a graphene edge. It is expected that these theoretical results give a clue to develop a new functional materials in industrial development phase.

Computational Details

In this work, we applied density functional theory (DFT) calculations with projector-augmented plane wave basis functions to edged-graphene. Our DFT studies used the Perdew-Burke-Ernzerhof (PBE) functional and exchange-correlation interactions under the generalized gradient approximations (GGA) frameworks. The wave-functions cutoff energy and the charge density cutoff energy were 30 and 240 Ry, respectively. The k-points mesh generation scheme used Monkhorst-Pack special point. All calculations of this study were carried out using the DFT program package of PHASE/0. The actual performance of the present version of PHASE showed 0.770 TFLOPS using 4 nodes of the Earth Simulator.

Keywords: Density functional theory, First-principles calculations, Graphene, Oxygen reduction reaction, Hydrogen evolution reaction