Search for Advanced Functional Materials concern with Eco-products

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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 files and so on. For applications of these electronic devices, we have interested in the feature of electronic structures of the graphenes. In particular this project, we focus upon work functions of the graphene surface and its affections of Nitrogen substitutions.

The electronic structure calculation was carried out based on density functional theory with PBE96 formulation for the exchange-correlation energy functional. The simulation used a model system, which consists of single-layered graphene-ribbon under the three-dimensional periodic boundary condition. The atomic positions of graphene-ribbons (with/without Nitrogen substitutions) were determined by the first-principles molecular dynamics methods. Actual performance of the present version of PHASE (Ver. 9.00) showed 0.770 TFLOPS using 4 nodes of the Earth Simulator.

In this work using the Earth Simulator, we obtained the following results of understanding affections of Nitrogen substitutions on the work function of graphene-ribbon.

1. When Nitrogen substitutes in the zigzag-edge position of graphene-ribbon, the work functions are lower values than other sites in graphene-ribbons.
2. However, when Nitrogen substitutes with pyridine-type in the zigzag-edge sites of graphene-ribbon, the work function does not show a reduction.

Keywords: Graphite, Graphene, Zigzag-edge, Work Function, Density Functional Theory Calculations