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 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 electronic structures of the armchair-edged graphene and its affections for nitrogen substitutions.

The electronic structure calculation was carried out based on density functional theory with a 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 from the graphene sheet structure by the DFT calculation. 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 the electronic structure changes of armchair graphene with a pyrridine like nitrogen-substitution:

1. For the only pyridinium substitution at the armchair-edge, the conduction band of the electronic density of state (DOS) does not obviously differ from the DOS of pure-graphene with armchair edge.
2. The structural stability of the nitrogen substituted graphene is decreased since the forming 6-members ring including the N-C-N (pyridinium) connections.
3. In the case of the substitution of quaternary nitrogen nearby a pyridinium nitrogen, a localized electronic state exist at the Fermi level.
4. For the localized electronic state in the case of the substitutions of pyridinium nitrogen and quaternary nitrogen, the correlated charge density to that electronic state localize at the armchair edge including the nitrogen. Particularly, there electrons localize at the carbon atoms

nearby pyridinium nitrogen, which looks like the zigzag edge graphene.

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

Keywords: Graphite, Graphene, armchair-edge, Nitrogen, Density Functional Theory Calculations