Functional Nano-Particles Simulation

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Abstract

In this study, we focus on the work-function in order to obtain any knowledge about contact resistance between metal and graphene. There is a piece of knowledge about the work functions of graphene[1]. However, it is so hard for experimental investigations to grasp a detailed understanding of its some elements substituted affection. We are concerned with this substitution effect of Nitrogen or Boron. Additionally, the effects of substitution position of Nitrogen atoms are investigated at low Nitrogen concentration.

Our calculations were carried out on the following conditions. 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 the two model systems, which were the 4×4 supercell containing 32 carbon atoms for 2D graphene-sheet structure and the 5×5 supercell containing 50 atoms for 1D graphene-ribbon structure. Actual performance of the present version of PHASE (Ver. 9.00) showed 0.770 TFLOPS using 4 nodes of the Earth Simulator.

Our results show the work-functions decreased by 20% at 3.125 atom% of Nitrogen in comparison with no substituted graphene, while it increase by 20% at 3.125 atom% Boron substituted graphene. And, we also obtain some useful knowledge as following from this work. Under the condition of two Nitrogen substitutions, the configurations of two Nitrogen-atoms giving low work-function provide some energy band in conduction band region shifts in valence band region. These distributions curve across the Fermi level at M-point.

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

Keywords: Graphene, Work function, the First-principles density functional theory calculation, Substitution

Reference:

[1] H. Hibino, H. Kageshima, M. Kotsugi, F. Maeda, F.-Z. Guo, Y. Watanabe, *Phys. Rev. B* **79**, 125437 (2009).