Ab initio study on electron-transport properties of graphene sheet depending on transport length

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Abstract

We perform *ab initio* studies on the electron-transport properties of graphene sheet sandwiched between semi-infinite electrodes. The transport properties of graphene depending on the sheet length and the vacancy density are numerically investigated. The π orbitals of carbon atoms play a main role in the electron transport. In the graphene sheet with a vacancy, the dangling bonds arising from the vacancy give rise to the contributions of σ orbitals to the transport, which are reduced as the sheet length becomes longer.

Introduction

Carbon-based nanomaterials attract much attention not only in the fields of physics, chemistry and electronics, but also in those of biology and life science. Graphene is one of carbon-based nanomaterials, which has a two-dimensional honeycomb structure and a single atomic layer of graphite, and is promising for application to nanoelectronics devices. Therefore, to understand the structural and electronic properties of graphene is very important. One of the present authors has analyzed the effects of defects in the graphene on the electron transport[1]. In this study, the dependence of the electron-transport properties on the length of spatial transport path and the density of defects are examined using first-principles calculations.

Computational Scheme

Our computational scheme is based on the real-space finite-difference (RSFD) method[2] within the framework of the density functional theory. The exchange-correlation effects are treated by the local spin density approximation and the interaction between electrons and atomic cores is described by the norm-conserving pseudopotentials of Troullier and Martins. To determine the Kohn-Sham effective

potential, a conventional supercell is employed under the periodic boundary condition in all directions. The graphene sheet is sandwiched between semi-infinite Au jellium electrodes and the transport properties are calculated by the overbridging boundary-matching method. The graphene sheets with different lengths in the transport direction are adopted to examine the zigzag-direction electron transport. The grid spacing is set to be 0.46 a.u., and the distances between the graphene strip and electrodes are taken to be 2.8 a.u.

Results and Discussions

In the calculation, the length of the grapehene sheet is varied between 7.0 a.u. and 20.9 a.u., and one carbon atom in the sheet is replaced by an atomic vacancy (Fig. 1). We examine the effects of the transport length and the density of vacancy on the transport properties. As the result, the spin polarization in the electronic structure is observed around the vacancy and the transport properties are affected by the spin of conducting electrons. In the cases of the
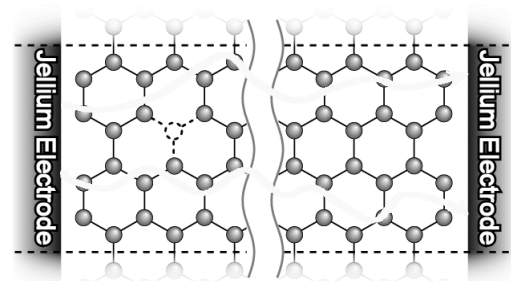

Fig. 1: Graphene sheet with a vacancy suspended between semi-infinite Au jellium electrodes. The dashed lines indicate the boundaries of conventional supercell.

models without the vacancy, the π orbitals of carbon atoms mainly contribute to the electron transport and the σ orbitals play secondary roles. On the other hand, for the models with the vacancy, the dangling bonds around the vacancy consisting of σ orbitals (sp^2 hybridized orbitals) also contribute to the electron transport when the transport length is short. However, as the transport length becomes longer, the contributions of dangling bonds rapidly decay. The details of this study are presented at the symposium

References

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