Optik - International Journal for Light and Electron Optics 206 (2020) 163755

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

Electronic structure and optical characteristics of AA stacked bilayer graphene: A first principles calculations

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ARTICLE INFO

Keywords:
Bilayer graphene
Optical spectra
Electronic structure
Electronic devices

ABSTRACT

First-principle calculations based on full potential linearized augmented plane-wave method have been performed to investigate the electronic and optical properties of 1×1 and 2×2 supercells of non-Bernal AA stacked bilayer graphene. The exchange-correlation effects in the present work have been treated using the local density approximation which show good agreement of the calculated structural and electronic properties with previous reports. From the calculated electronic properties, semimetallic nature is found for 1×1 supercell of bilayer graphene, while a pseudogap is observed for the 2×2 supercell. Our results indicate that the pseudogap in 2×2 supercell of bilayer graphene originates from the increased number of valence and conduction band states contributing in the electronic structure of this configuration and suppressing the states in the vicinity of Fermi level. In order to understand the effects of non-Bernal AA stacking of two graphene layers on the optical response, we have computed the optical properties in terms of complex dielectric function for electromagnetic radiations having polarization vectors parallel and perpendicular to the *xy*-plane. Our calculated optical properties show a significant enhancement of optical absorption of electromagnetic radiations having polarization vector parallel to *xy*-plane, which is ascribed to the augmentation of 2D honeycomb lattice of carbon atoms in form of bilayer graphene. These results highlight tunable electronic and optical characteristics of graphene that might prove advantageous for its employment in electronic devices.

1. Introduction

In recent past the low-dimensional polymorphs of carbon namely: fullerenes [1], carbon nanotubes [2], carbon graphene [3], and carbon nanoribbons [4,5] have been intensely scrutinized due to their propitious applications in post-silicon nano-electronic devices.

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https://doi.org/10.1016/j.ijleo.2019.163755
Received 21 July 2019; Received in revised form 18 October 2019; Accepted 7 November 2019