Investigation of the electronic, magnetic and optical properties of navol carbon allotrope

Samira Kazemi*, Rostam Moradian

Physics Department, Faculty of Science, Razi University, Kermanshah, Iran

Received: 30.03.2017 Final revised: 08.04.2018 Accepted: 07.05.2018

Abstract

In this paper, we investigate triple properties of monolayer pentagon graphene that include electronic, magnetic and optical properties. Our research based on density functional theory (DFT) and the WIEN2k computational code is done. Our results show that in the electronic and magnetic properties, this structure with a direct gap energy of about 2.2 eV along $\Gamma \rightarrow \Gamma$ direction and total magnetic moment of 0.0013 μ_B per unit cell is almost a non-magnetic semiconductor. Also, in the optical properties, the variation of optical parameters including dielectric constant, loss energy function and reflectivity in term of energy are drawn and studied. Its optical properties show that if this allotrope is used in solar cell technology, its efficiency in the low energy will be better, because its loss energy function and reflectivity will be minimum.

Keywords: Density functional theory, monolayer pentagon, density of states, electronic bandstructure, Optical properties.

* Corresponding author: samirakazemi1234@gmail.com