Effect of adsorption h-BN nano layer on the electronic and structural properties of WS_2 monolayer by using first-principles study

Seyyed Fardin Taghizadeh*,[1], Zahra Ghasemi majd[1], Peiman Amiri[2], Behrooz Vaseghi[1]

[1]Department of Physics,college of Science, Yasouj University, Yasouj 75914-353, Iran

[2]Department of Physics, College of Science, Shahid Chamran University of Ahvaz, Ahvaz, Iran

Received: 25.10.2017 Final revised: 21.07.2018 Accepted: 22.10.2018

Abstract

The adsorption of h-BN monolayer on WS2 nano sheet was studied following the framework of density functional theory using Quantum ESPRESSO package. First-principle calculations with different exchange-correlation functionals including LDA, GGA, semi-empirical and ab-initio van der Waals in the forms of DFT-D2, vdW-DF2B86R and vdW-DF2 have been performed to evaluate the performance of different functionals in describing bonding mechanism, adsorption energy and interlayer distance of WS_2 monolayer on h-BN layer. In order to include the van der Waals (vdW) interactions in our calculations, we used the DFT-D2 and vdW methods and found the vdW-DF2B86R seems to be the most qualified approach. Both vdW and semi-empirical methods predict a physical adsorption with no net charge transfer between the WS_2 layer and the corresponding substrates. In addition, we investigated the electronic and structural properties and density of states of WS_2 and h-BN heterolayers by vdW-DF2B86R functional. Based on our calculations, WS_2/h-BN heterostructure show a direct band gap at the K-point, which has been experimentally observed.

Keywords: Adsorption, Boron nitride, Electronic structure, First-principle calculations, Tungsten disulfide, van der Waals interaction

* Corresponding Author: Taghizadeh@yu.ac.ir