ABSTRACT

Tungsten Disulfide (WS_2) is a two-dimensional material known for its tunable electronic properties that depend on the number of atomic layers. This study aims to analyze the differences in the electronic properties of WS_2 in monolayer and bilayer configurations using a theoretical approach based on Density Functional Theory (DFT). The initial structure of WS_2 was obtained from the Materials Project database and converted into Quantum ESPRESSO input files using the Burai interface. The converted structures were then tested for convergence with respect to cut-off energy and k-point mesh. Simulations were carried out using the Self-Consistent Field (SCF) and Non-Self-Consistent Field (NSCF) methods to compute the band structure and Density of States (DOS). The results show that monolayer WS_2 exhibits a direct bandgap of approximately 1.823 eV at the K point, while bilayer WS_2 exhibits an indirect bandgap of 1.593 eV due to interlayer coupling. In addition, the energy bandgap in bilayer WS_2 was found to be lower than in the monolayer configuration. These distinctions in electronic behavior provide valuable insight for tailoring WS_2 as a functional material for optoelectronic applications such as photodetectors and light-emitting devices.

Keywords: *WS_2, monolayer, bilayer, Density Functional Theory, bandgap, Density of States, optoelectronics*

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