

## 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

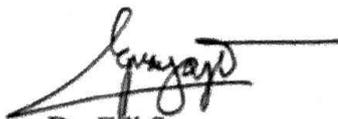
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Dosen Pembimbing I,



Vincensius G. S. K., S.Si., M.Si., Ph.D  
NIP. 197105221997021001

Dosen Pembimbing II,



Dr. Edi Suprayoga  
NIP. 198804082019021003