ABSTRACT

The band gap of molybdenum disulfide (MoS_2) monolayer undergoes a direct-to-indirect transition under uniaxial strain influence. It is evidenced by the wavelength shift and the increasing intensity of the photoluminescence experiment along with greater value of uniaxial strain applied on MoS_2 monolayer. Theoretically, the band gap value of MoS_2 monolayer decreases along with the increasing of applied strain and has a direct-to-indirect band gap transition at a strain of $\sim 1\%$. *Meanwhile, the semiconductor-to-metal transition occurs at strain value of* $\sim 10\%$. *The physical reasons behind the direct-to-indirect band gap transition have been discussed variously and are open for further investigation. This study has conducted ab initio calculation which implements the density functional theory (DFT) method using Quantum ESPRESSO package to obtain the electronic band structure, density of states (DOS), and projected DOS (PDOS) of MoS_2 monolayer under uniaxial strain influence. The uniaxial strain value is varied from* $0 - 2.8\%$ *with* 0.2% *step along a crystallographic axis. This study found that the direct-to-indirect band gap transition on MoS_2 monolayer occurs due to the shifting of electron density from adjacent to sulfur towards molybdenum. This transition is proved to have correlation with the DOS contribution alteration of each orientation for Mo-*$4d$ *and S-*$3p$ *orbital. Raman spectra calculation of the unstrained MoS_2 monolayer has also been conducted despite has not been able to have a good agreement with the experiment results. The* E' *Raman mode occurs at* $384\ \mathrm{cm}^{-1}$ *while the* $A_1{}'$ *mode at* $414\ \mathrm{cm}^{-1}$.

Keywords**:** *MoS_2, Monolayer, Uniaxial strain, Ab initio calculation, DFT method, Electronic band structure, density of states, Quantum ESPRESSO.*