ABSTRACT

Semiconductor materials are dominant in the fabrication of electronic devices. Unlike metals, the presence of an energy band gap makes them ideal for application in optoelectronics nanostructures. Silicon was the most preferred 2D material to be used, but due to its limitations, for example, quantum tunneling effects, graphene was preferred to silicon. However, graphene has no bandgap, and since the bandgap property is very useful in electronics, research is ongoing to replace silicon and graphene with Transition Metal Dichalcogenides (TMDs). TMDs make nanostructures easily with adjustable energy bandgap, hence applicable in optoelectronics. They exhibit various unique optoelectronic characteristics, attracting interest due to distinct features from bulk predecessors and have bandgap characteristics between 1.80 - 2.30 eV, which can be tuned to fabricate Field Effect Transistors (FET) and other optoelectronic devices. Molybdenum disulfide has sparked attention among TMDs because of the potential of tuning the band gap. Up to date, research on the effects of impurities and pressure on the energy band gap of molybdenum disulfide have been studied, resulting in energy band gaps falling between 1.3 - 1.55 eV. There is need to reduce the value of the energy band gap further so as to make the semiconductor applicable at lower energies. Therefore, this study combined the ionic doping and pressure application on MoS_2 in an attempt to narrow the energy band gap to a lower value that could accommodate majority of radiations falling under electromagnetic spectrum. Structural optimization of MoS_2 monolayer and niobium doped MoS_2 was done using the Density Functional Theory (DFT) method as implemented by the Quantum ESPRESSO simulation package. The study utilized PBE-GGA method of approximation and the number of k-points utilized were 8 x 8 x 1. The structure was optimized to a cell dimension of 3.175 Å for $a = b$ parameters. A vacuum height of 14.971 Å served to minimize artificial interactions between periodic layers. A 4 x 4 x 1 supercell was modelled and had optimized dimensions of 12.57 Å for $a = b$ and a vacuum height of 14.971 Å. Its band gap energy was found to be 1.70 eV. Upon 8.33% niobium doping of the 4 x 4 x 1 MoS_2 supercell, the energy band gap reduced to 1.375 eV. A pressure in the range of -2.852 GPa to 6.832 GPa was applied, which corresponds to strains ranging from 2. 52 % to -2.50 %. The energy band gap for undoped MoS_2 monolayer reduced from 1.70 eV to 1.40 eV at a pressure of -2.852 GPa. The energy band gap for the 8.33% Nb doped MoS_2 monolayer narrowed from 1.375 eV to 1.25 eV at a pressure of -5.166 GPa. The combined effect decreased the band gap of MoS_2 monolayer from 1.70 eV to 1.25 eV. This study concludes that the combined effect of Nb doping and pressure on the structure of molybdenum disulfide can improve its electronic properties by reducing its energy band gap. This property makes it useful in fabricating optoelectronic devices which can work well at lower energies.