Strain-induced modulation of 2D transition metal dichalcogenides homo and heterostructure: Prediction from computational approach

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The ultimate goal of this research work using density functional theory calculations, the electronic properties, magnetic and phonon band structure of two-dimensional (2D) bilayer systems of transition metal dichalcogenides (TMD) investigated. Some of TMDs investigated for the biaxial tensile and compressive strain on homo and hetero structure of NbX2 (X = S, Se, Te) influenced by magnetism with a ferromagnetic character cause of the focused impacts of through-bond interaction and also through-space interaction. In whole mechanism of the system, 4d orbital of Nb transition atom play significant role of this exchange on transition of spin moment concept. The raised magnetic moments have been remarkable increased or decreased by the tensile and compressive strain, even affecting a half-metallic and semiconductor properties by the strong spin polarization near the Fermi level. We assume that our calculated outputs might suitable for spintronics related technologies such as memory and quantum-computer devices are considerable. This would light up a new direction to find out the spintronics in two-dimensional nanostructures.

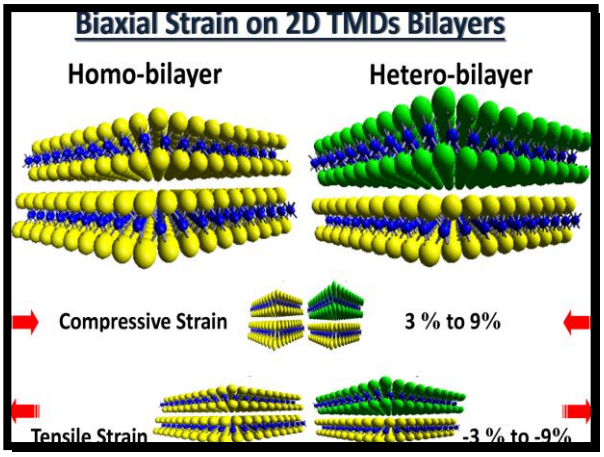

Figure 1. Depicted the figure of Homo and Hetero bilayer and biaxial strain on Niobium dichalcogenides systems

[1] Y.Zhou, et al., ACS Nano, 6, 2012
[2] M. Sharma, et al., J. App. Phys. 116, 2014

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