# Strain-Engineered MoS2/WS2 and XS2/VS2 (X=Mo, W) Heterostructures for Hydrogen Generation and Spintronics Applications

**R.Thangavel and Saurav Lahiri,** *Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad, Jharkhand 826004, India*

rthangavel@iitism.ac.in

Abstract

Innovative semiconductor heterostructures, MoS2/WS2 and XS2/VS2 (X=Mo, W), offer promising solutions for solar energy-driven hydrogen generation and advanced opto-spintronics applications. This study comprehensively examines their structural, electronic, photocatalytic, and magnetic properties under biaxial strain using density functional theory (DFT) and Monte Carlo (MC) simulations. The MoS2/WS2 heterobilayer, with its most stable stacking configuration (conf-1), shows a low interlayer binding energy of −18.07 meV/Å² and type II band alignments, which enhance charge carrier mobility and reduce recombination rates. This heterostructure also exhibits superior visible light absorption ($8.3 \times 10^5$ cm$^{-1}$) compared to its monolayers. Its band positions under tensile and compressive strains are suitable for hydrogen evolution (HER) and oxygen evolution reactions (OER), highlighting its potential for water-splitting applications. The strain-induced red shifts in absorption edges further indicate its capability for efficient solar energy harvesting. Concurrently, the XS2/VS2 heterostructures reveal notable ferromagnetic properties, with indirect band gaps and type II heterojunctions ideal for opto-spintronics devices. They maintain high Curie temperatures (TC) of 299.08 K (MoS2/VS2) and 301 K (WS2/VS2) as determined by MC simulations. While the WS2/VS2 heterostructure transitions to a half-metal under tensile strain beyond 1%, both heterostructures retain their semiconducting nature under other strains. This strain-induced tunability of electronic and magnetic properties underscores their versatility for customized device applications. These findings pave the way for further exploration of 2D van der Waals heterostructures in hydrogen generation and opto-spintronics. Strain engineering emerges as a critical tool for optimizing their performance, suggesting a wide range of potential applications in energy and technology sectors.

## References

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[2] Saurav Lahiri and R. Thangavel, Modulation of magnetic properties of trilayer MoS2/ZnO/VS2 van der Waals heterostructure via strain engineering for spintronics application. Physics Letters A 522 (2024) 129764. DOI: j.physleta.2024.129764

[3] Yichuan Chenab and Mengtao Sun Nanoscale, 13, (2021 )5594-5619, https://doi.org/10.1039/D1NR00455G

## Figures

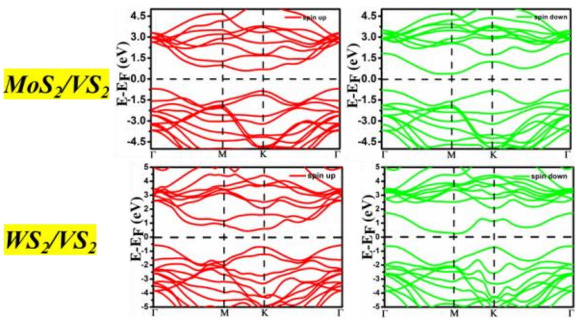


**Figure 1:** HSE Spin polarized band structure for (a) spin up (b) spin down channel of MoS2/VS2 while (c) spin up and (d) spin down of WS2/VS2 heterostructure

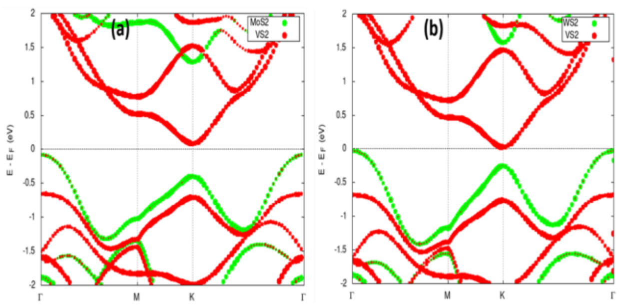


**Figure 2:** PBE+U computed projected band structure of (a) MoS2/VS2 and (b) WS2/VS2 heterostructure