**ABSTRACT**

Graphene and two-dimensional materials based on transition metal dichalcogenides have gained increasing attention because of their fascinating features in electronics and optical properties [1]. Combining single-layer of graphene with a transition metal dichalcogenides layer in Van der Waals heterostructures offers an intriguing means of controlling the electronic properties through these bilayer heterostructures [2]. Here, we report the structural and electronic properties of the graphene/MoS₂ bilayer heterostructures. For theoretical study calculations, we used density functional theory (DFT) with Van der Waals corrections [3]. We analyse the interlayer spacing between the graphene/MoS₂ layers, the relaxed position of atoms and charge transfer between the layers. We focused on the optimised bilayer heterostructures with different supercell geometries (4:3, 5:4 and 9:7), having different magnitudes of lattice mismatch.

**METHODOLOGY:**

- **ABINIT** [3] is the software that was employed to carry out the DFT calculations.
- Bilayer separation distance calculations.
- Relaxation (Atomic positions and geometries are modified).
- Report the structural and electronic properties.
- With and without spin orbit coupling (SOC).
- Different pseudopotentials [HGH(NCPP), GGA-PW+VdW and LDA].

**RESULTS**

Graphene/MoS₂, bi layer 4:3 [Graphene(4X4)/ MoS₂ (3X3)]

- After relaxation Mo₃ layer is stretched and graphene layer is compressed.
- Distance between Mo layer and graphene layer (Z) is 4.872 Å.
- S varies ∆Z≈0.0132 Å.
- The Fermi level is shifted and graphene layer is compressed.
- Electric properties of the Dirac point can change.

Graphene/MoS₂, bi layer 5:4 [Graphene(5X5)/ MoS₂ (4X4)]

- After relaxation Mo₃ layer is compressed and graphene layer is stretched.
- Distance between Mo layer and graphene layer (Z) is 4.672 Å.
- Mo layer and graphene layer are shifted.
- MoS₂ bilayer heterostructure.
- Spin orbit coupling effect.

Graphene/MoS₂, bi layer 9:7 [Graphene(9X9)/ MoS₂ (7X7)]

- After relaxation Mo₃ layer was very small compression and graphene layer was large.
- Distance between Mo layer and graphene layer (Z) is 4.338 Å.
- Mo layer and graphene layer are shifted.
- MoS₂ bilayer heterostructure.
- Spin orbit coupling effect.

**REFERENCES**