Metallicity at heterojunctions of semi-conducting Transition Metal Dichalcogenides.

Sridevi Krishnamurthi
Dr. Geert Brocks

Computational Materials Science, Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, the Netherlands.
s.krishnamurthi@utwente.nl

Figures

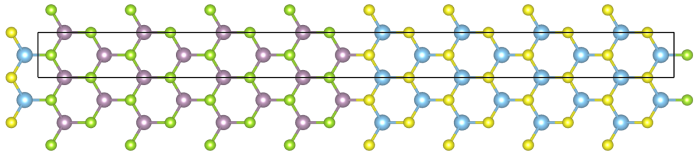

Figure 1: A Unit cell of a lateral heterostructure made of semi-conducting TMDCs

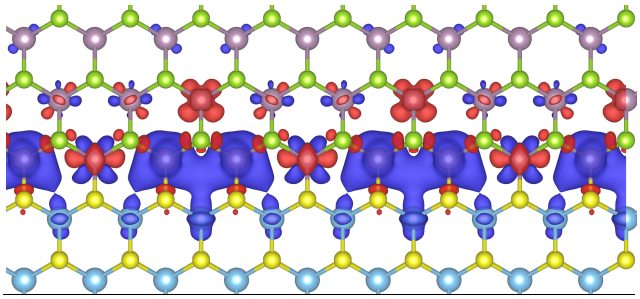

Figure 2: Charge density wave at the interface that causes a bandgap opening.

Abstract

Lateral monolayer heterostructures from transition metal dichalcogenides (TMDCs) have been studied both by experiments and by calculations in recent times. Semiconducting TMDC layers of D_{3h} symmetry have the bulk polarisation as a topological invariant. With DFT calculations We show that, if two semi-conducting monolayers of different polarisations are put together laterally, metallic edge states appear along the interface. These 1-d interface states, although protected by crystal symmetry, are subject to charge and spin density wave instabilities that then lead to the opening of a bandgap.

References

[1] R. D. King-Smith and David Vanderbilt, Phys. Rev. B **47**, (1993) ,1651(R)

[2] Fang, Chen and Gilbert, Matthew J. and Bernevig, B. Andrei, Phys. Rev. B.**86**, (2012) 115112