Boron phosphide based 2D heterostructures

Yesim MOGULKOC[1]
Aybey MOGULKOC[2] and Mohsen MODARRESI[3]
[1]*Department of Physics Engineering, Faculty of Engineering, Ankara University, Ankara, Turkey*
[2]*Department of Physics, Faculty of Science, Ankara University, Ankara, Turkey*
[3]*Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran*

mogulkoc@eng.ankara.edu.tr

Abstract

With fascinating physical properties of the van der Waals (vdW) heterostructures are emerging as promising materials for future possible optoelectronic devices. Motivated by the recent studies on vdW heterostructures, we investigate the electronic and optical properties of boron phosphide based 2D heterostructures that we especially focused on the monolayer boron phosphide (MBOP)/monolayer blue phosphorus (MBP) and monolayer gallium nitride (MGaN)/monolayer boron phosphide (MBOP) in the framework of density functional theory (DFT). We analyze the variation of the energy band gap, the characteristics of the energy band diagrams, charge redistribution by stacking and the electrostatic potential along the perpendicular direction. The dynamical stability of these structures is ensured by the phonon spectra. We conclude that the heterostructures have remarkable optical absorption over the UV range together with being transparent to the visible spectrum, and may be a prominent material for future optoelectronic devices.

REFERENCES

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[2] A. Mogulkoc, Y. Mogulkoc, M. Modarresi, and B. Alkan, Phys.Chem.Chem.Phys., 20 (2018) 28124.

FIGURES

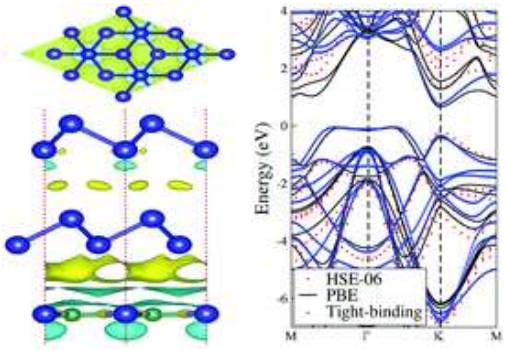

Figure 1: MBOP/MBP heterostructures [1]

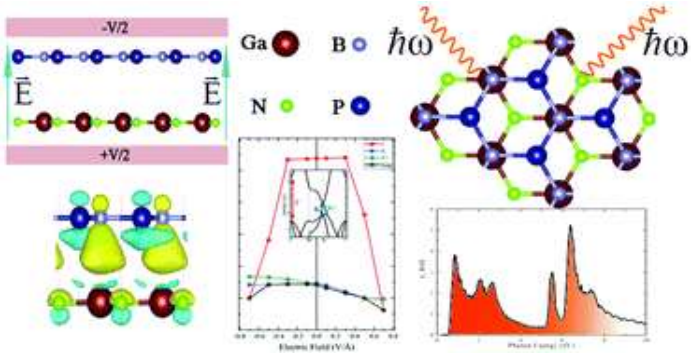

Figure 2:. MGaN/MBOP heterostructures [2]