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Boron phosphide based 2D heterostructures

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MOTIVATION

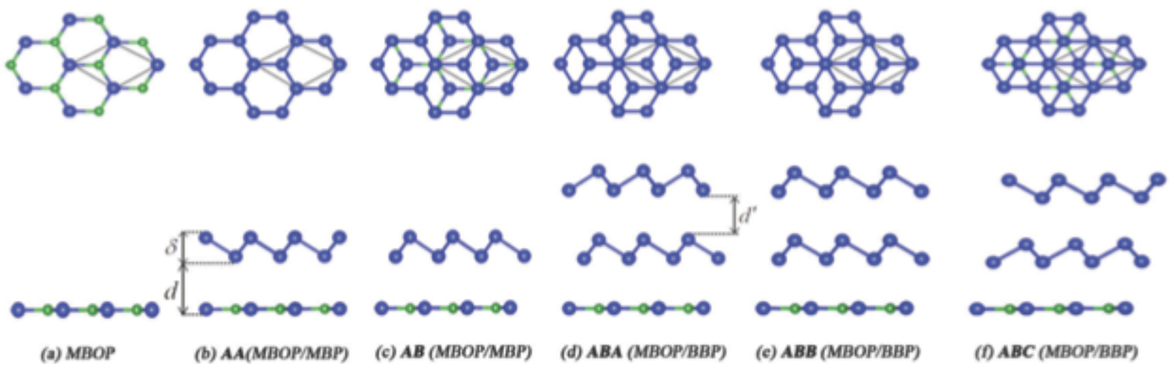
- With the **down-sizing of devices** in the electronics industry, 2D layered materials have become the focus of experimental and theoretical work due to their low dimensional interface properties.
- Designing alternative versatile 2D heterostructures improve electronic and optical properties compared with monolayer 2D materials due to the **mutual interaction between the layers**.
- Boron phosphide has **superior carrier mobility** (over 10^4 cm^2 V^{-1} s^{-1}).
- Band gaps are changing according to the layers.

METHOD

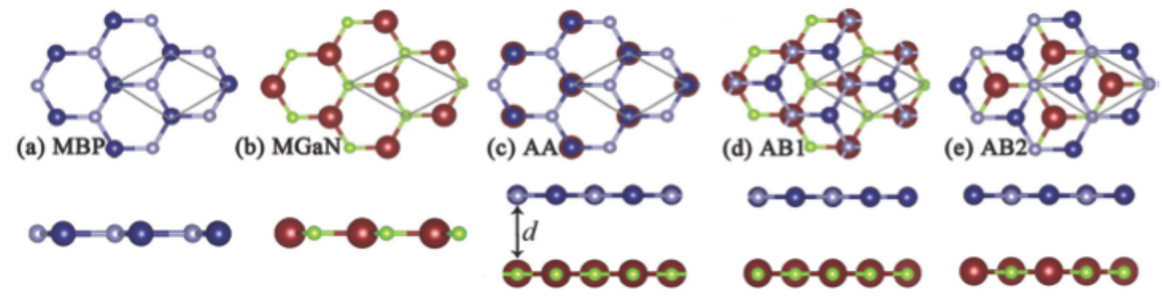
- First-principles calculations are based on density functional theory **(DFT)** performed by **VASP** package.
- The exchange–correlation potentials are approximated by the generalized gradient approximation **(GGA)** with the Perdew– Burke–Ernzerhof **(PBE)** and hybrid Heyd–Scuseria–Ernzerhof **(HSE06)** functionals.
- The van der Waals interaction is important for layered hetero- structures which is taken into account by the **DFT-D2** method.

Geometrical Structures

Monolayer boron phosphide/blue phosphorus heterostructures

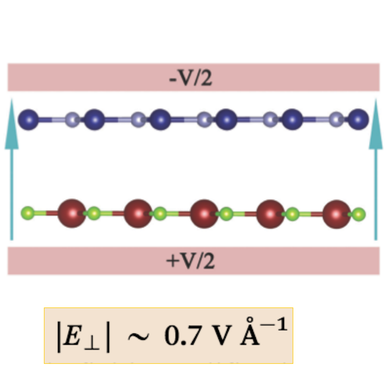


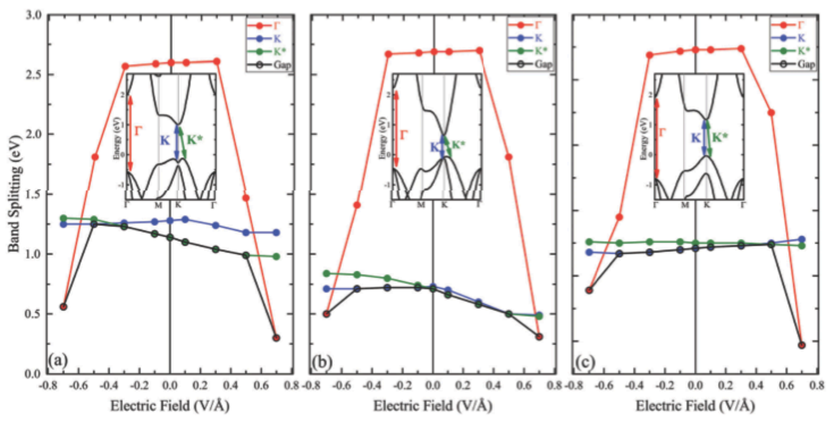
GaN/boron phosphide heterostructures



Electric Field Effect

GaN/boron phosphide heterostructures





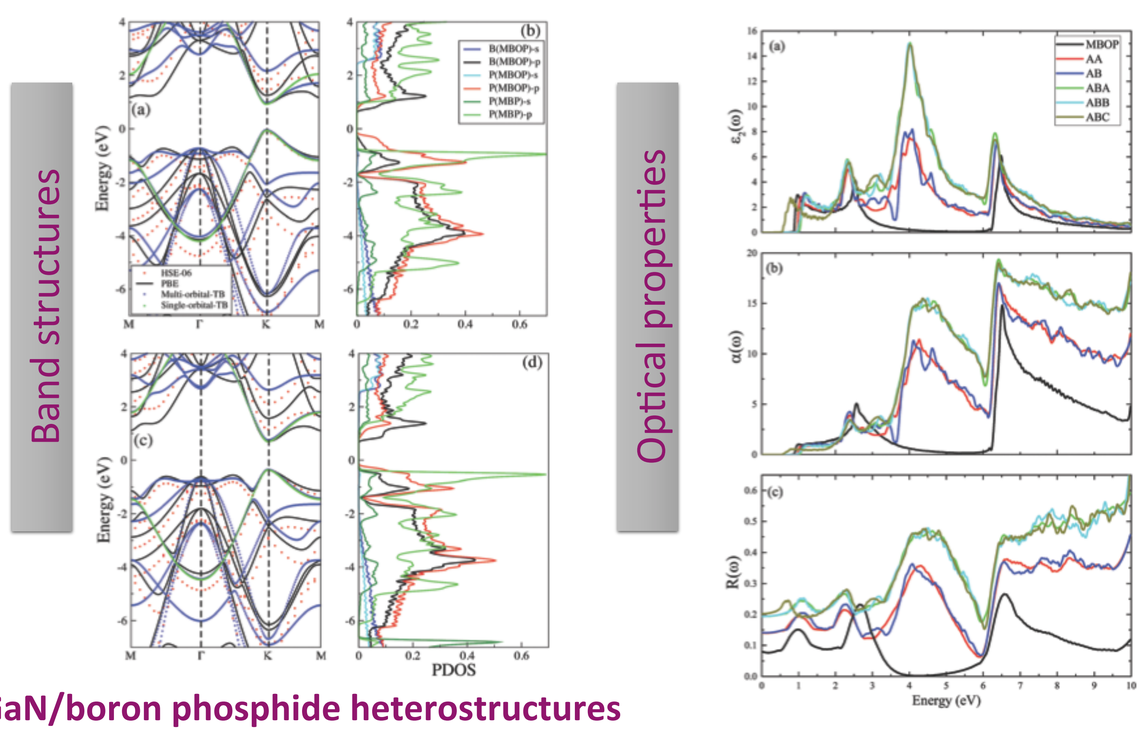
SCOPE

- We analyze **the variation of the energy band gap**, the characteristics of the energy band diagram of the boron based 2D systems which are **boron phosphide/blue phosphorus** and **GaN/boron phosphide** heterostructures.
- We examine the **optical properties** of monolayer boron phosphide and heterostructures as part of DFT calculations.
- We have also analyzed these properties under the external **electric field**.

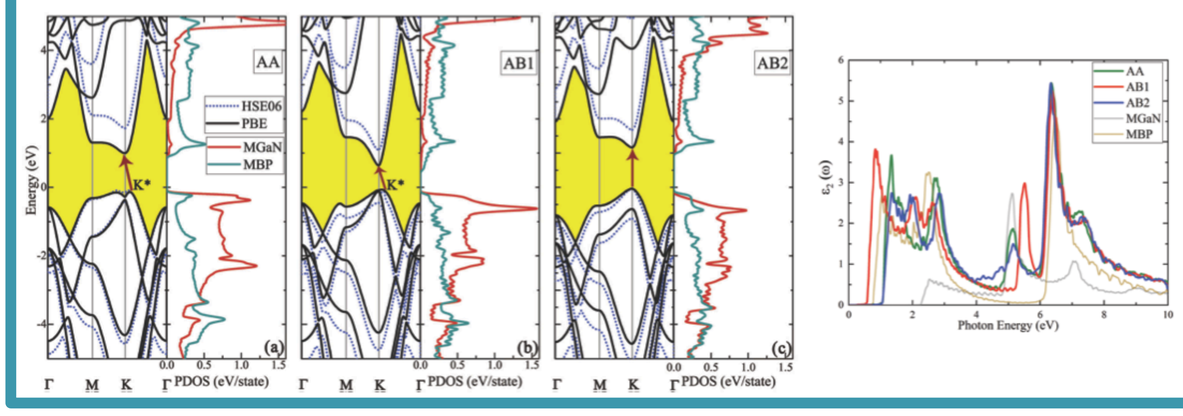
? Can we recommend boron phosphide based 2D heterostructures for optoelectronic applications?

Electronic & Optical Properties

Monolayer boron phosphide/blue phosphorus heterostructures



GaN/boron phosphide heterostructures



CONCLUSIONS

- All of the heterostructures that are proposed are found to be stable by considering the phonon spectra.
- Pristine MBP has an indirect energy band gap, and heterobilayers of MBOP/MBP have direct band gaps.
- For the MGaN/MBOP system, while AA and AB1 are found to be indirect band gap semiconductors, AB2 has a direct band gap where the MBP layer dominates the band structure.
- Finally, we examined the optical properties of the heterostructures by considering the frequency dependent imaginary dielectric function.
- It is also seen that the prominent optical absorption of the heterobilayers arises from the UV range, promising for optoelectronic applications based on the UV spectral region.

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2. A. Mogulkoc, Y. Mogulkoc, M. Modarresi, and B. Alkan, ”Electronic structure and optical properties of novel monolayer gallium nitride and boron phosphide heterobilayers”, *Phys.Chem.Chem.Phys.,* 2018, 20, 28124.

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