A first principle study of shifted, twisted and tilted hBN/BP bilayers

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Among the family of 2D materials, black phosphorus (BP) has singular characteristics including an anisotropic structure, a direct gap tuneable on a wide range of energies, and a remarkable hole conductivity [1].

However, BP thin films are very reactive, so they must be protected (e.g. with capping layers) in order to be integrated in real devices. Hexagonal boron nitride (hBN), has shown to constitute exceptionally good capping material by virtue of its extreme flatness and large band gap [2].

Because of these reasons, it makes sense to investigate the properties of heterostructures formed of BP and hBN. In this work, we address this subject by scrutinizing from first principle the structural (stability and strain distribution) and electronic properties of many free-standing hBN/BP bilayers with different configurations. We will discuss the changes in electronic and stability properties when one layer is shifted on top of the other (traslations), when is twisting (angle mismatch), and when the BP layer is tilted (as in the structure studied by [3]).

References

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Figures

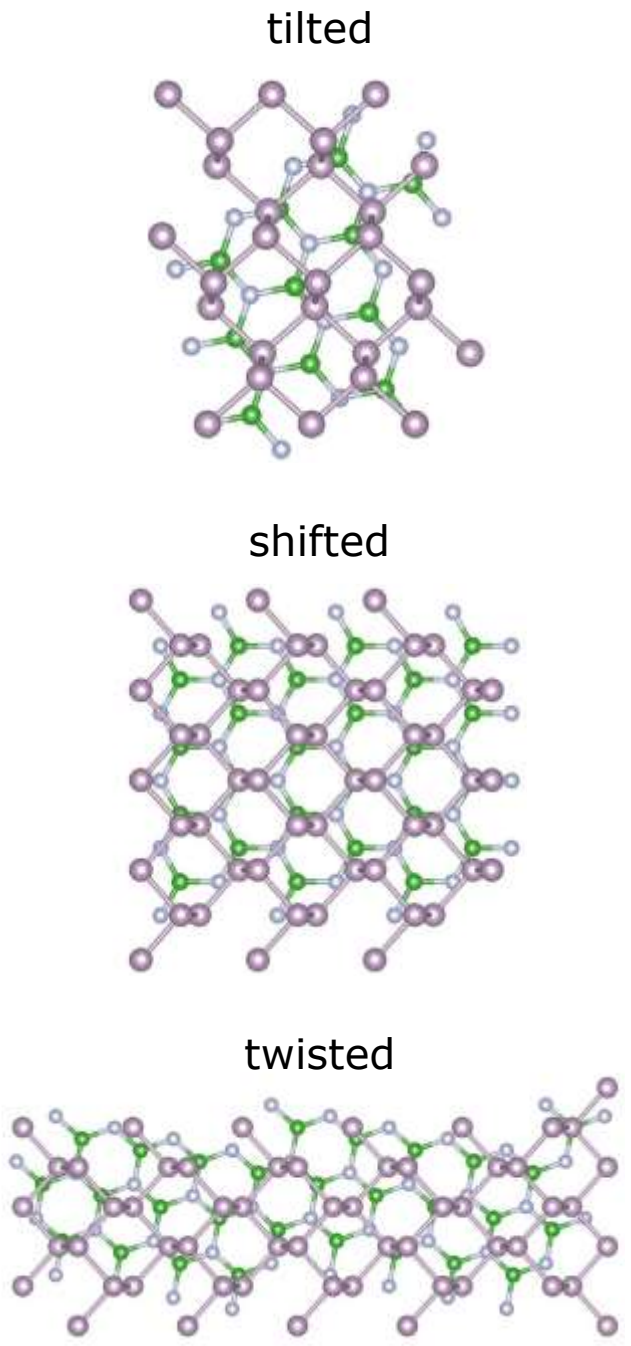

Figure 1: Three configurations of the hBN/BP bilayer explored in this study.