First-principles study of structural and electronic properties of graphene/MoS_2 heterostructure

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One of the most well-known two-dimensional heterostructures is the graphene/MoS_2, which was successfully synthesized in experiments [1], consisting of MoS_2 with stronger spin-orbit coupling (SOC) than pristine graphene. Meanwhile, this fact makes the combination of both structures allow us to combine both material's outstanding properties, including ultrahigh mobility and spin transport lengths in graphene and spin-orbitronic phenomena coupled to valleys in MoS_2 [2]. Recent studies proved strong SOC is obtained by graphene in the graphene/MoS_2 heterostructure, which is also theoretically promising for optospintronics [3,4]. These explanations promoted the reason for the importance of research in this field. It is desirable to tune the electronic structure by external field, doping, and defect. In the present work, we first thoroughly investigate the relationship between geometry and electronic properties of the heterostructure by emphasizing the interlayer spacing. Even though there are some experimental and theoretical studies about this heterostructure, we are trying to remodel 4×4 graphene and 3×3 MoS_2 (4:3 configuration) supercell and investigate the effect of various interlayer distances between graphene and MoS_2 to provide a broader analysis of the structural and electronic properties of the heterostructure. This study was carried out by giving some variations of interlayer distance value. The research is performed by the full-potential linearized augmented plane wave (FLAPW) method using generalized gradient approximation (GGA). The supercell is made up of 59 atoms of graphene and MoS_2 in total. As the result of introducing different interlayer spacing, various structural and electronic properties are acquired. The optimized configuration consists of 3.38% lattice mismatch between two materials which have six-fold symmetries. The bond length between C atoms is 1.42 Å, while the bond length of Mo-Mo atoms is 3.28 Å, agreed with the previous study [5]. In the band structure, Dirac point originated in graphene is found near the Fermi level, in which a small gap, typically ~0.1 meV, is introduced by the weak hybridization to MoS_2. The bandgap in the Dirac point is increasing as the interlayer spacing is decreasing. However, different interlayer spacing resulted in the various bandgap values. Whereas electronic properties experienced some changes, the interlayer distance modification does not significantly affect the bond lengths of graphene and MoS_2 in the supercell. A comprehensive and detailed discussion of the results and comparison with the previous study of structural and electronic properties of graphene/MoS_2 heterostructure is presented.

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