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Effects of electric field on the electronic structures of MoS_2/arsenene van der Waals heterostructure

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ABSTRACT

Electronic structures modulation in MoS_2/arsenene van der Waals(vdW) heterostructure with an external electric field(E_{ext}) are investigated by density functional theory(DFT). It is demonstrated that the MoS_2/arsenene heterobilayer is a type-II vdW heterostructure, and therefore electrons and holes are spatially separated. The band gap of MoS_2/arsenene is significantly modulated by E_{ext}, eventually a transition from semiconductor to metal occurs. The positive and negative E_{ext} have different effects on the band gap due to the spontaneous electric polarization in MoS_2/arsenene heterostructure. The variation of band edges as a function of E_{ext} provides further insight to the linear variation of the band gap. Furthermore, the MoS_2/arsenene vdW heterostructure experiences transitions from type-II to type-I and then to type-II under various external electric fields. The E_{ext} can control not only the amount of charge transfer but also the direction of charge transfer at the MoS_2/arsenene interface. The present study would open a new avenue for application of ultrathin MoS_2/arsenene heterojuction in future nano- and optoelectronics.

Keywords: band alignment; electric field; band gap; MoS_2/arsenene vdW heterostructure

1. Introduction

Two-dimensional (2D) materials have great potential in next-generation photonic and electronic applications owing to their outstanding fundamental physical properties and extensive applications [1-5]. In spite of being a very promising 2D material, gapless graphene has limitation in optoelectronics and nanoelectronics applications [6–9]. As [1]alternatives, new researches have emerged focusing on other 2D materials such as transition metal sulfides (TMDs) [10-12]. MoS_2, one typical representative member of

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