Arsenene-based heterostructures: high-efficient bifunctional materials for photovoltaics and photocatalytics

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To explore the influence of vdW on band edges of heterostructures, we take As/TCNQ heterostructure as an example. The (3×4) supercell of arsenene was used to minimize the constraint induced by the periodic boundary model. Spin-polarization and dipole correction were employed to cancel the errors in total energy, electrostatic potential and atomic force, caused by periodic boundary condition. vdW interaction was included by the DFT-D2 level.

As clearly shown in Figure S1, the vdW interaction has very limited influences on the band structure in As/TCNQ heterostructure. The CBM of As/TCNQ is mainly composed by TCNQ, while the VBM is composed by arsenene and both of them are very similar to the isolated results except very small shifts in band edges. More importantly, the band edges from both methods are not that big. Considering GW calculations are unaffordable for large sized heterostructure supercells and the current scheme can in principle reflect the intrinsic nature of heterostructures, we employed the isolated calculations as a compromise.

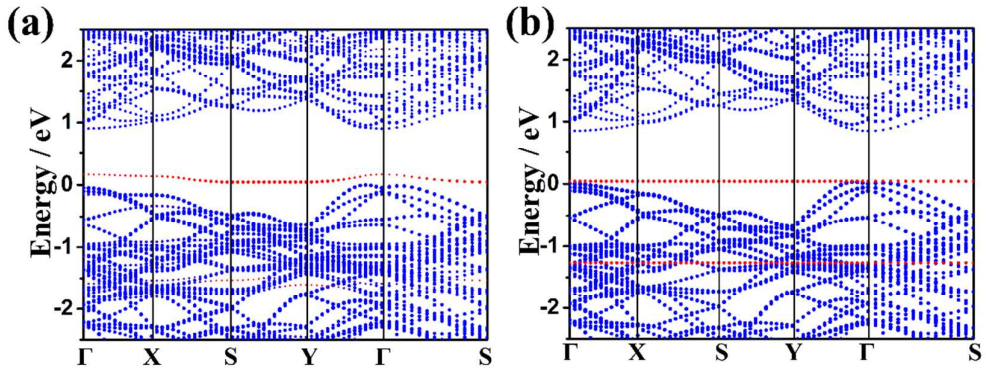

Figure S1: Band structure of (a) As/TCNQ heterostructure, (b) isolated calculation of arsenene and TCNQ based on GGA+PBE. The bands plotted in blue and red indicate the bands dominated by arsenene and TCNQ layer, respectively. The vacuum levels are aligned and the Fermi level is set as zero.

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