Supplementary material

Arsenene/$Ca(OH)_2$ van der Waals heterostructure: Strain tunable electronic and photocatalytic properties

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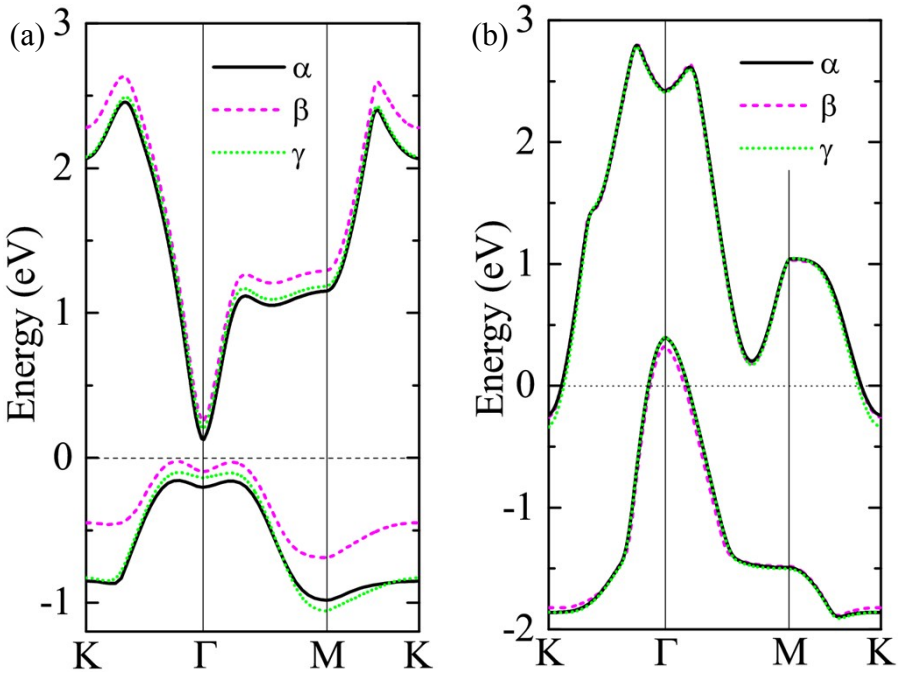

Fig. S1. (Color online) The evolutions of the highest valence bands and the lowest conduction bands of the A/C heterostructures with α-, β-, and γ-stacking under (a) +10% tensile and (b) -10% compressive biaxial strains, respectively.

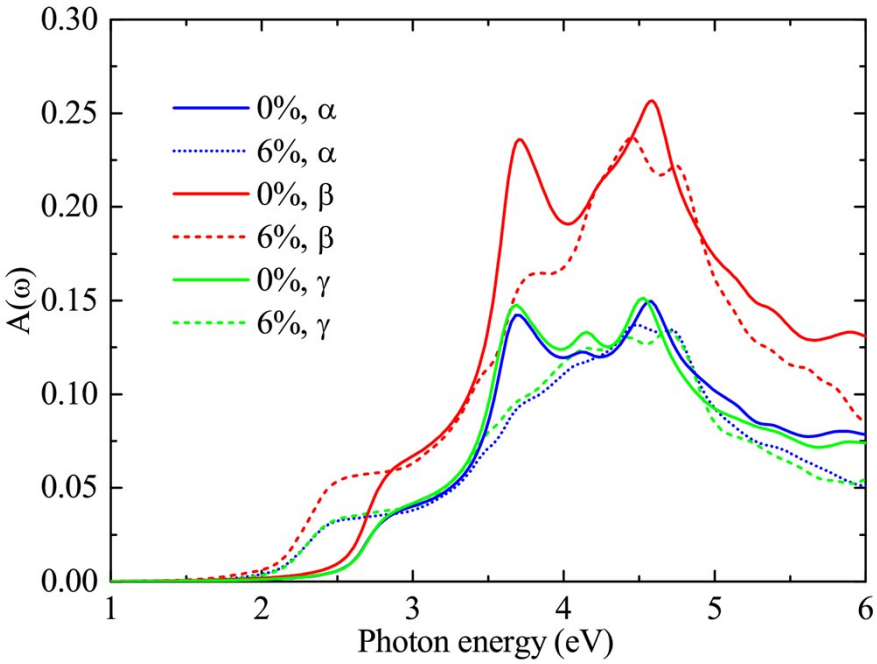

Fig.S2. (Color online) The optical absorbance spectrum A(ω) of A/C heterostructure with α-, β-, and γ-stacking at the strains of 0% and +6%. A(ω) is calculated using the PBE functional followed by a rigid energy shift to take into account the bandgap underestimation of the PBE functional.