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Bandgap engineering and charge separation in two-dimensional GaS-based van der Waals heterostructures for photocatalytic water splitting

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Abstract

Two-dimensional (2D) gallium sulfide(GaS), hexagonal boron nitride (h-BN) and graphitic carbon nitride (g-C_3N_4) have been fabricated and expected to be promising photocatalysts under ultraviolet irradiation. Here we employ hybrid density functional calculations to explore the potential of the 2D GaS-based heterojunctions GaS/h-BN (g-C_3N_4) for the design of efficient water redox photocatalysts. Both heterostructures can be formed via van der Waals (vdW) interaction and are direct bandgap semiconductors, whose bandgaps are reduced comparing with isolated GaS, h-BN or g-C_3N_4 monolayers and whose band-edges straddle water redox potentials. Furthermore, the optical absorption of GaS/h-BN (g-C_3N_4) heterostructures is observably enhanced in the ultraviolet-visible (UV-VIS) light range. The electron-hole pairs in GaS/h-BN (g-C_3N_4) heterostructures are completely separated from different layers. In addition, the in-plane biaxial strain can effectively modulate the electronic properties of GaS/h-BN(g-C_3N_4) heterostructures. Thus the GaS/h-BN (g-C_3N_4) heterostructures are anticipated to be promising candidates for photocatalytic water splitting to produce hydrogen.

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