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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-C₃N₄) 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-C₃N₄) 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-C₃N₄ monolayers and whose band-edges straddle water redox potentials. Furthermore, the optical absorption of GaS/h-BN (g-C₃N₄) heterostructures is observably enhanced in the ultraviolet-visible (UV-VIS) light range. The electron-hole pairs in GaS/h-BN (g-C₃N₄) 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-C₃N₄) heterostructures. Thus the GaS/h-BN (g-C₃N₄) heterostructures are anticipated to be promising candidates for photocatalytic water splitting to produce hydrogen.

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