Electronic Supplementary Information

Efficient band structure tuning, charge separation, visible-light response in ZrS$_2$-based van der Waals heterostructures†

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Fig. S1 Charge distribution of pure ZrS$_2$ monolayer. The charge densities of the VB (blue) and CB (red) is plotted with an isovalue of 0.02 e/Å$^3$.

Fig. S2 Charge density differences of hybrid h-BN/ZrS$_2$ heterostructure compared with the isolated ZrS$_2$ and graphene monolayers. Pink, blue, yellow and dark green balls represent B, N, S and Zr atoms, respectively. Blue and red isosurfaces represent, respectively, charge accumulation and depletion in the space. The isovalue chosen to plot the isosurfaces is 0.0001 e/Å$^3$. 

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**Fig. S3** Charge density differences of hybrid g-C₃N₄/ZrS₂ heterostructure compared with the isolated ZrS₂ and graphene monolayers. Grey, blue, yellow and dark green balls represent C, N, S and Zr atoms, respectively. Blue and red isosurfaces represent, respectively, charge accumulation and depletion in the space. The isovalue chosen to plot the isosurfaces is 0.0001 e/Å³.

**Fig. S4** Charge density differences of hybrid PG/ZrS₂ heterostructure compared with the isolated ZrS₂ and graphene monolayers. Grey, white, yellow and dark green balls represent C, H, S and Zr atoms, respectively. Red and blue isosurfaces represent, respectively, charge accumulation and depletion in the space. The isovalue chosen to plot the isosurfaces is 0.0001 e/Å³.
Fig. S5 Fully relaxed structures. (a) Side view and top view of graphene/ZrS$_2$ heterostructure. (b) Side view and top view of h-BN/ZrS$_2$ heterostructure. (c) Side view and top view of g-C$_3$N$_4$/ZrS$_2$ heterostructure. (d) Side view and top view of PG/ZrS$_2$ heterostructure.