Electronic Supplementary Information

Efficient band structure tuning, charge separation, visible-light response in ZrS_2-based van der Waals heterostructures†

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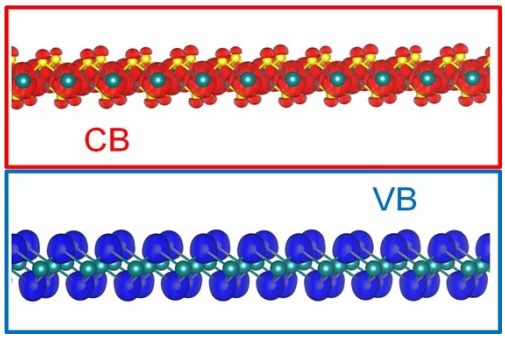

Fig. S1 Charge distribution of pure ZrS_2 monolayer. The charge densities of the VB (blue) and CB (red) is plotted with an isovalue of 0.02 e/Å^3.

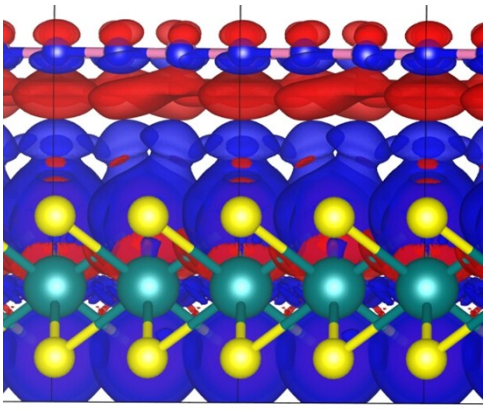

Fig. S2 Charge density differences of hybrid h-BN/ZrS_2 heterostructure compared with the isolated ZrS_2 and graphene monolayers. Pink, blue, yellow and dark green balls represent B, N, S and Zr atoms, respectively. Blue and red isosurfaces represent, respectively, charge accumulation and depletion in the space. The isovalue chosen to plot the isosurfaces is 0.0001 e/Å^3.

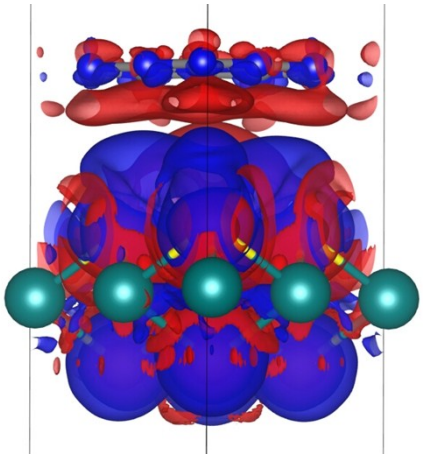

Fig. S3 Charge density differences of hybrid g-C_3N_4/ZrS_2 heterostructure compared with the isolated ZrS_2 and graphene monolayers. Grey, blue, yellow and dark green balls represent C, N, S and Zr atoms, respectively. Blue and red isosurfaces represent, respectively, charge accumulation and depletion in the space. The isovalue chosen to plot the isosurfaces is 0.0001 e/Å^3.

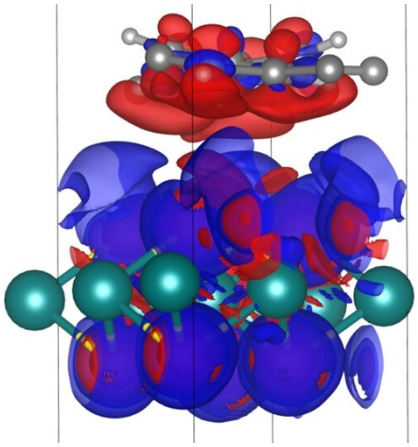

Fig. S4 Charge density differences of hybrid PG/ZrS_2 heterostructure compared with the isolated ZrS_2 and graphene monolayers. Grey, white, yellow and dark green balls represent C, H, S and Zr atoms, respectively. Red and blue isosurfaces represent, respectively, charge accumulation and depletion in the space. The isovalue chosen to plot the isosurfaces is 0.0001 e/Å^3.

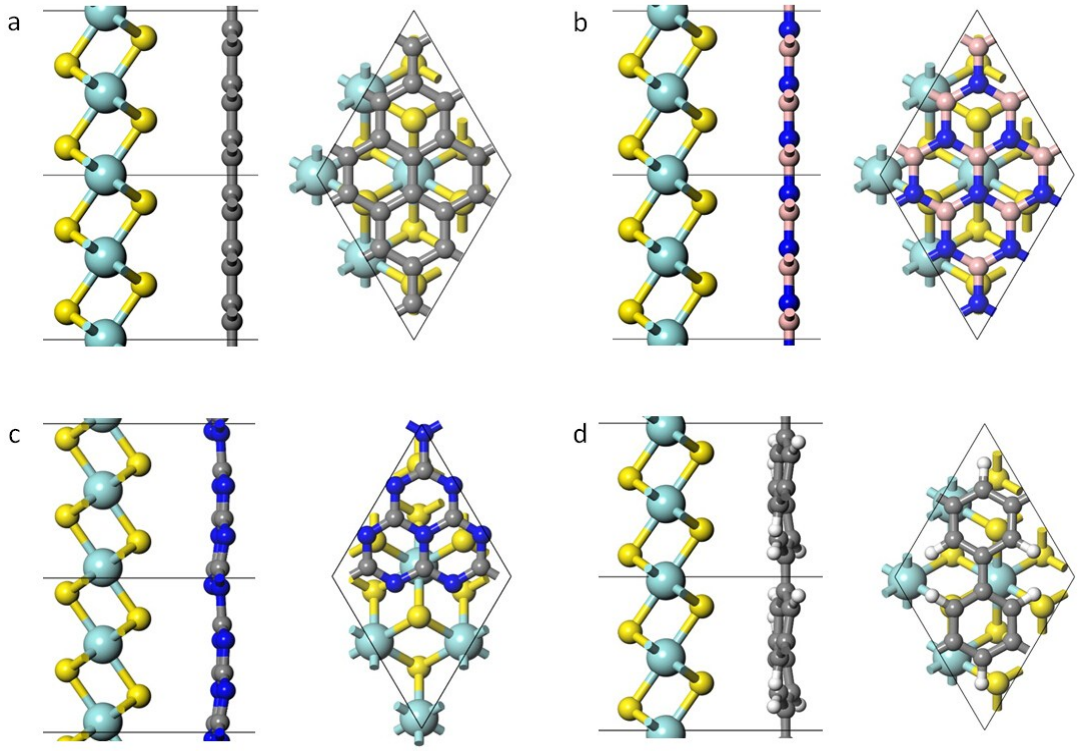

Fig. S5 Fully relaxed structures. (**a**) Side view and top view of graphene/ZrS_2 heterostructure. (**b**) Side view and top view of h-BN/ZrS_2 heterostructure. (**c**) Side view and top view of g-C_3N_4/ZrS_2 heterostructure. (**d**) Side view and top view of PG/ZrS_2 heterostructure.