Supplementary material

Influence of Vacancy Defects on the Interfacial Structural and Optoelectronic Properties of ZnO/ZnS Heterostructures for Photocatalysis

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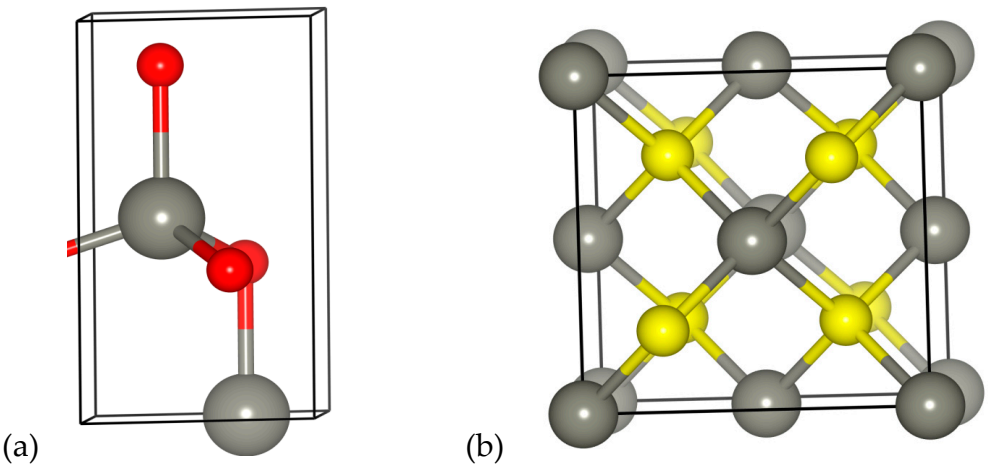
Figure S1. Optimized unit cells of (a) bulk wurtzite ZnO and (b) bulk cubic ZnS, where red, yellow and silver balls represent oxygen, sulfur and zinc atoms, respectively.

Figure S2. Optimized structures of (a) ZnO6L and (b) ZnS2L surfaces.

Figure S3. ZnO layers away from the interface, interface region and top ZnS layer of (a) perfect heterostructure, and heterostructures with (b) V_O, (c) V_S and (d) V_{Zn}, where red, yellow, silver, green, blue and black balls represent oxygen atom, sulfur atom, zinc atom, V_O, V_S and V_{Zn}, respectively.

Figure S4. Schematic diagram of band alignment for ZnS2L and ZnO6L before contact, versus normal hydrogen electrode potential.

Figure S1. HSE06 calculated band structures of (a) wurtzite ZnO and (b) cubic ZnS by using mixing exchange parameter of 0.375 and screening parameter of 0.20 $Å^{-1}$.



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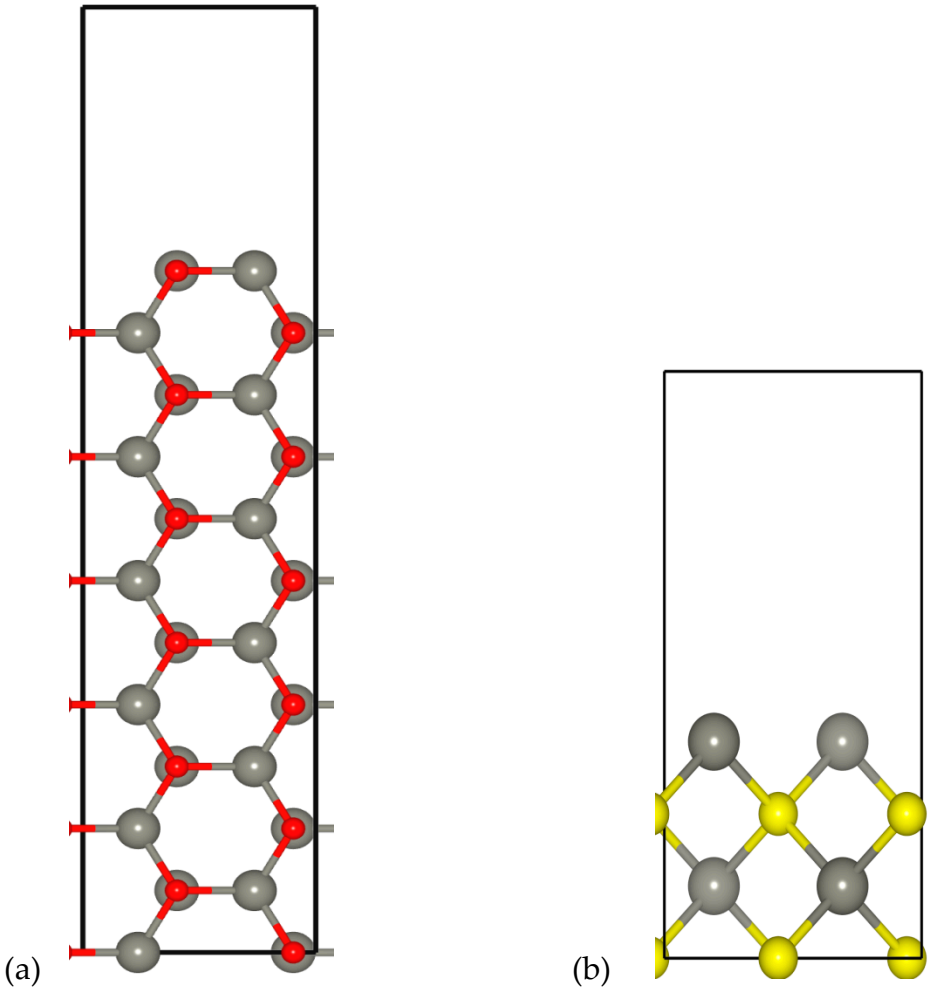
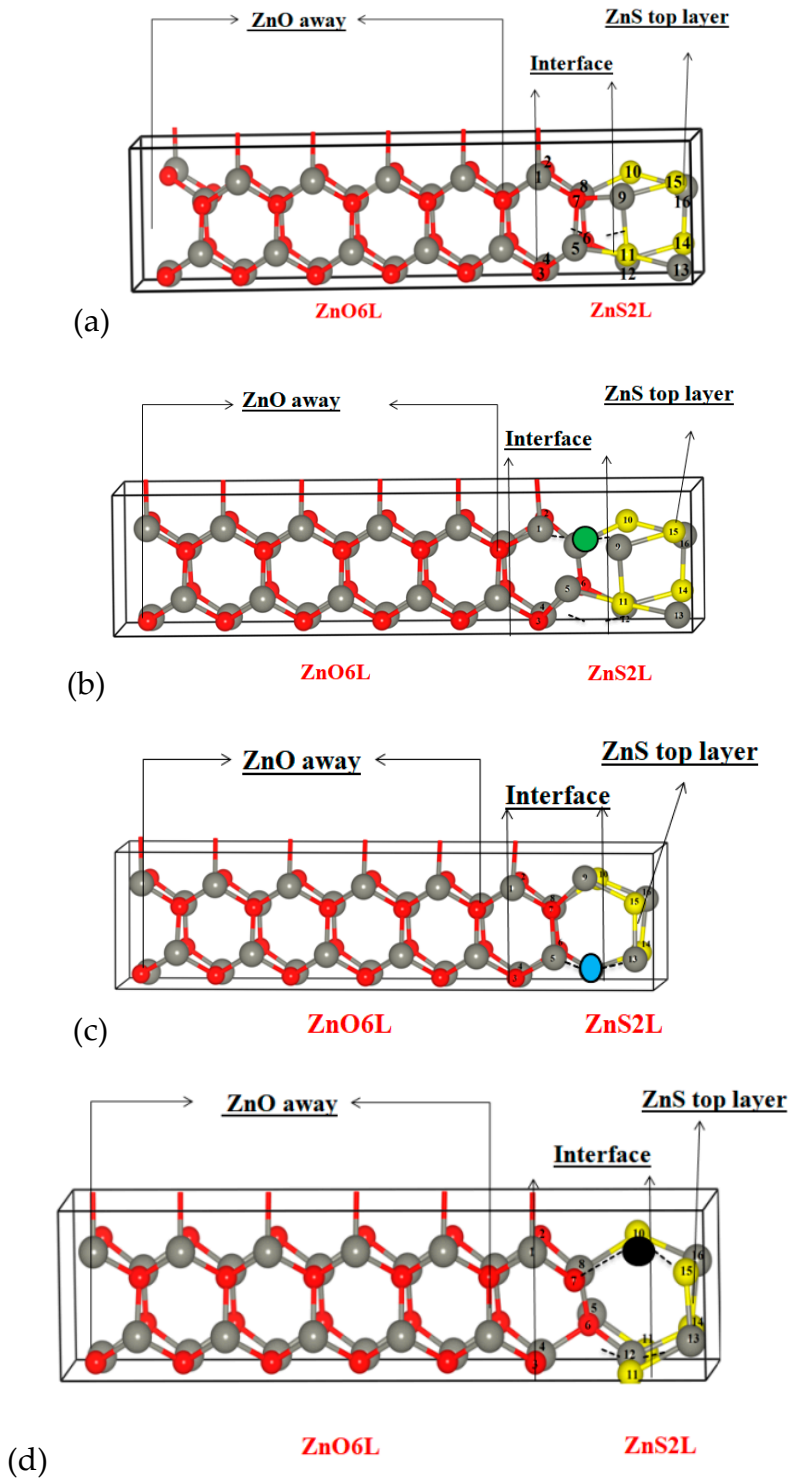


Figure S2. Optimized structures of (a) ZnO6L and (b) ZnS2L surfaces..



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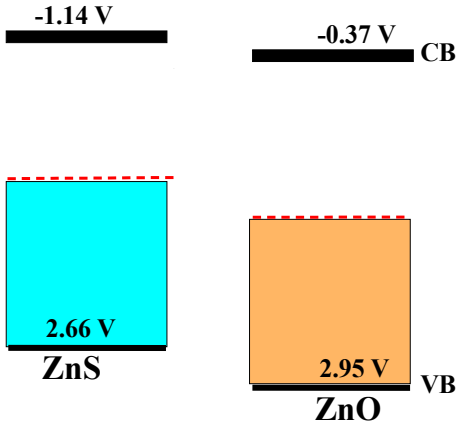

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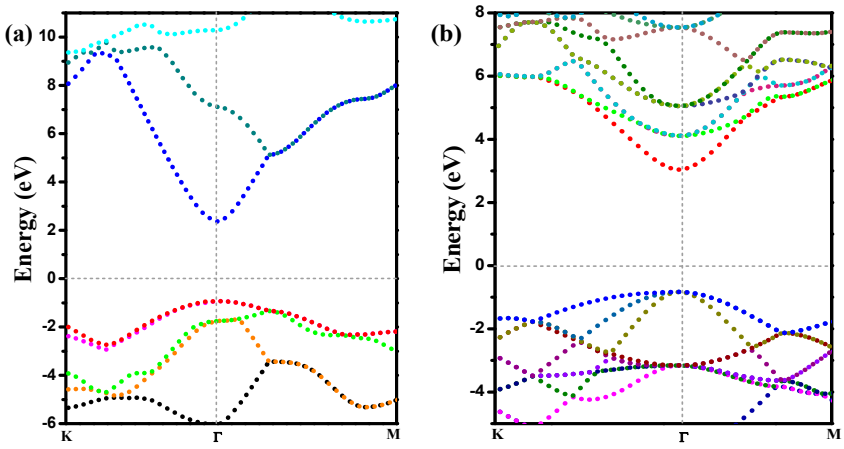

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