Electronic Supplementary Information (ESI)

ZnO-GaN Heterostructured Nanosheets for Solar Energy Harvesting: Computational Studies Based on Hybrid Density Functional Theory

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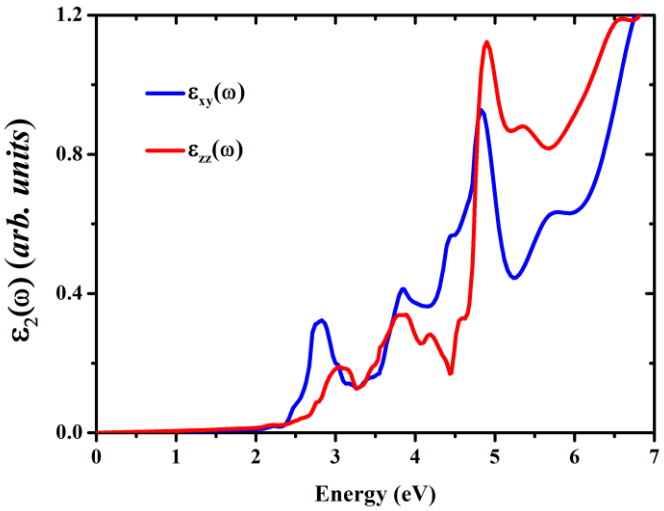

Figure S1 Imaginary part $\varepsilon_2(\omega)$ of the H-$(ZnO)_4(GaN)_4$ nanosheets.

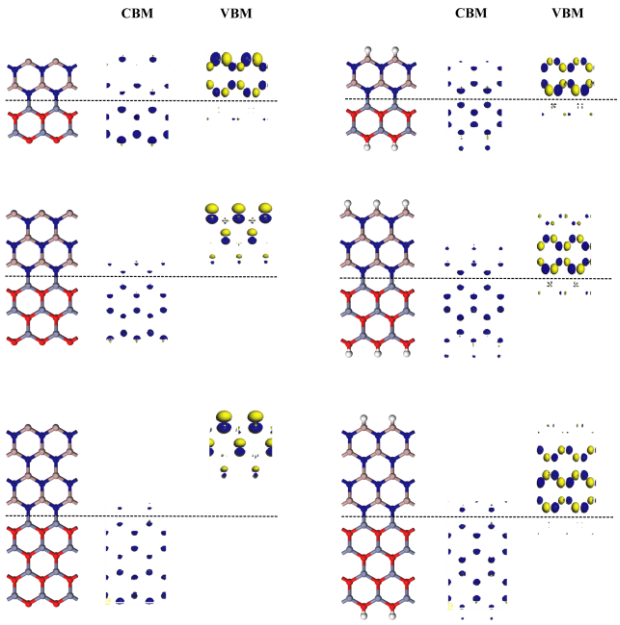

Figure S2 Charge distribution of the band edges for the bare (left) and hydrogenated (right) $(ZnO)_m(GaN)_n$ (m = n = 2, 3, 4) nanosheets, respectively. Black dashed lines represent the interface between the ZnO and GaN region.

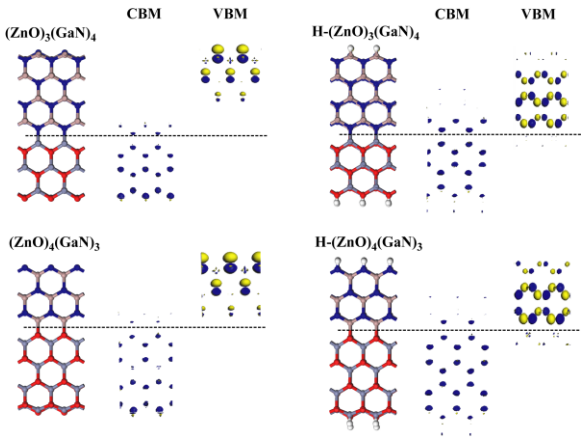

Figure S3. Charge distributions of the bare (left) and passivated (right) the $(ZnO)_3(GaN)_4$ and $(ZnO)_4(GaN)_3$ nanosheets. Black dashed lines represent the interface between the ZnO and GaN region.