**Electronic Supplementary Information**

# A direct Z-scheme photocatalyst $PtS_2/HfGe_2N_4$ van der Waals heterostructure for highly efficient water splitting: First-principles study

Wen Qiao*, Xinzhuo Zhang, Shiming Yan*, Ru Bai, Tiejun Zhou
School of Electronics and Information, Hangzhou Dianzi University, Hangzhou 310018, China

*Corresponding author:
E-mail address: qiaow@hdu.edu.cn (Wen Qiao), shimingyan@hdu.edu.cn (Shiming Yan).

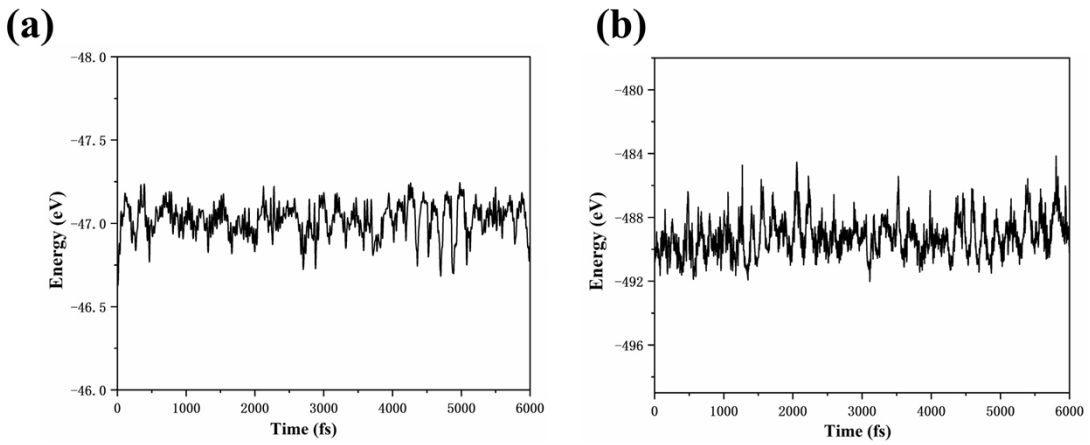


**Fig. S1.** The AIMD simulation at 300 K of $PtS_2$ (a) and $HfGe_2N_4$ (b)

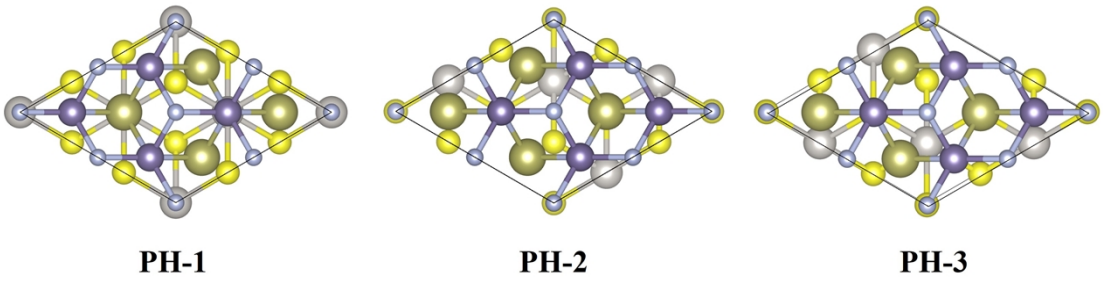


**Fig. S2.** The structures of $PtS_2/HfGe_2N_4$ heterostructures with different configurations.

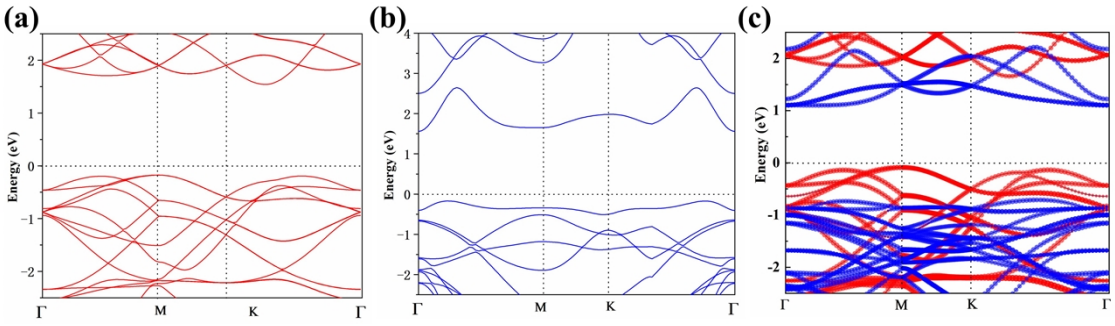


**Fig. S3.** Band structures of $\sqrt{3} \times \sqrt{3}$ supercell $PtS_2$ (a), a unit cell $HfGe_2N_4$ (b) and $PtS_2/HfGe_2N_4$ heterostructure (c) calculated using PBE functional.

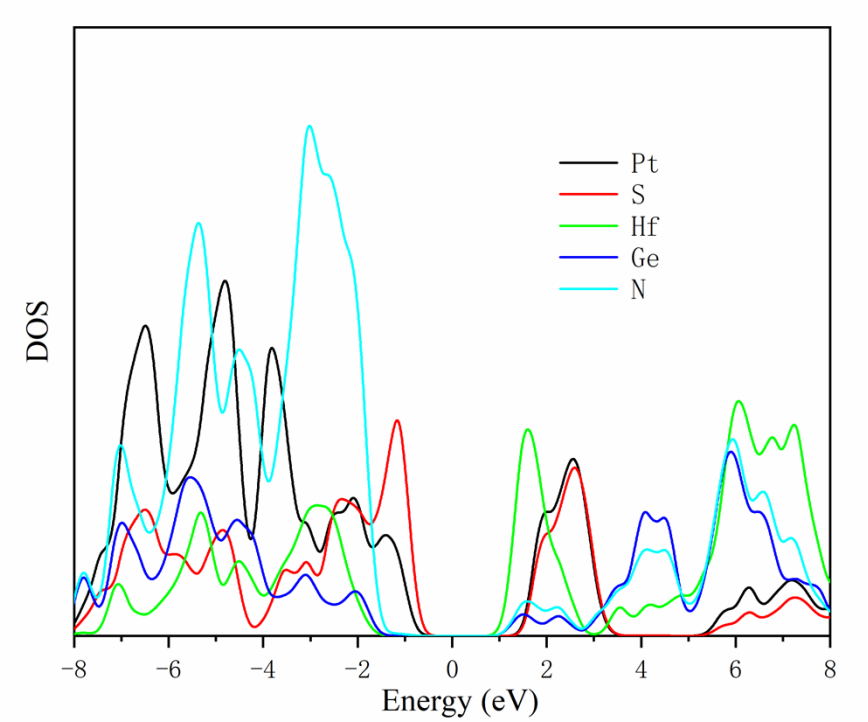


**Fig. S4.** Projected density of states of $PtS_2/HfGe_2N_4$ heterostructure.

**Table S1**

Calculated zero-pint energy correction ($E_{ZPE}$), entropy contribution (TS, T=298.15K), total energy (E).

| | $E_{ZPE}$ (eV) | -TS (eV) | E (eV) |
|---|---|---|---|
| * | / | / | -268.02 |
| *O | 0.08 | -0.06 | -272.04 |
| *OH | 0.37 | -0.09 | -276.30 |
| *OOH | 0.38 | -0.15 | -281.42 |
| *H | 0.19 | -0.03 | -270.71 |