Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

Monolayer $Ge_2Te_2P_4$ as promising photocatalyst for solar driven water-splitting: A DFT study

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AFFILIATIONS

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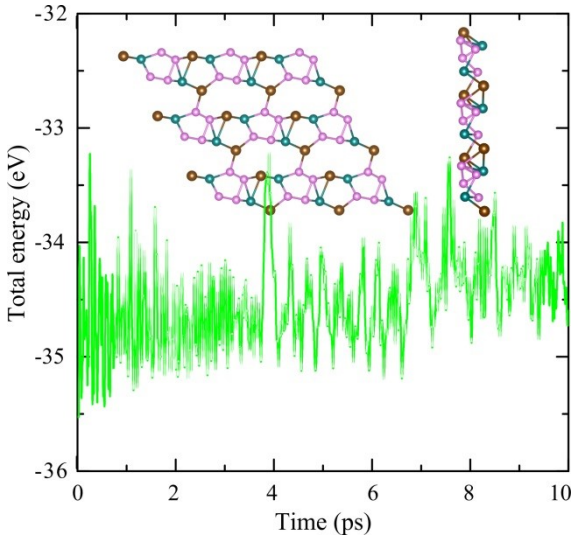

Fig. S1. The AIMD energy fluctuations at 900 K, and the snapshot of equilibrium structure of $Ge_2Te_2P_4$ monolayer after 10 ps.

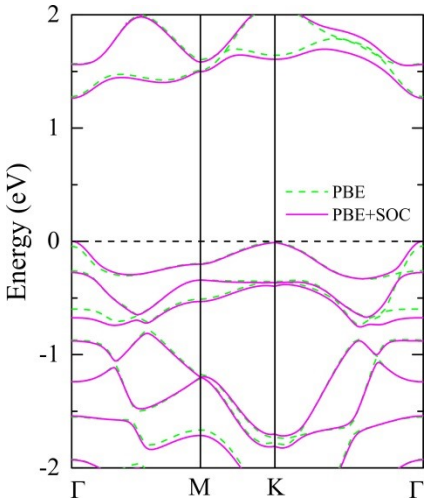

Fig. S2. The calculated electronic band structure of the $Ge_2Te_2P_4$ monolayer with spin-orbital coupling (SOC) (pink), and without SOC (dash green curves) extracted from PBE functional.

Table S1. The calculated Gibbs free energy ΔG_H via Grimme's D2 and D3 methods.

	Grimme's D2	Grimme's D3
Te-site	-1.78 eV	-1.86 eV
Ge-site	-2.45 eV	-2.54 eV
P-site	-2.61 eV	-2.71 eV