**Supplementary Information**

# Machine-Learning Prediction of Metal Sulfide Photocatalysts for Sacrificial Hydrogen Evolution under Visible Light Irradiation

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**Table S1** Conditions of convergence criteria for geometric optimization

| Self-consistent field tolerance / eV atom$^{-1}$ | Energy tolerance / eV atom$^{-1}$ | Maximum force tolerance / eV Å$^{-1}$ | Displacement tolerance / Å | Max stress / GPa |
|---|---|---|---|---|
| $1.0\times10^{-6}$ | $1.0\times10^{-5}$ | 0.03 | $1\times10^{-3}$ | 0.1 |

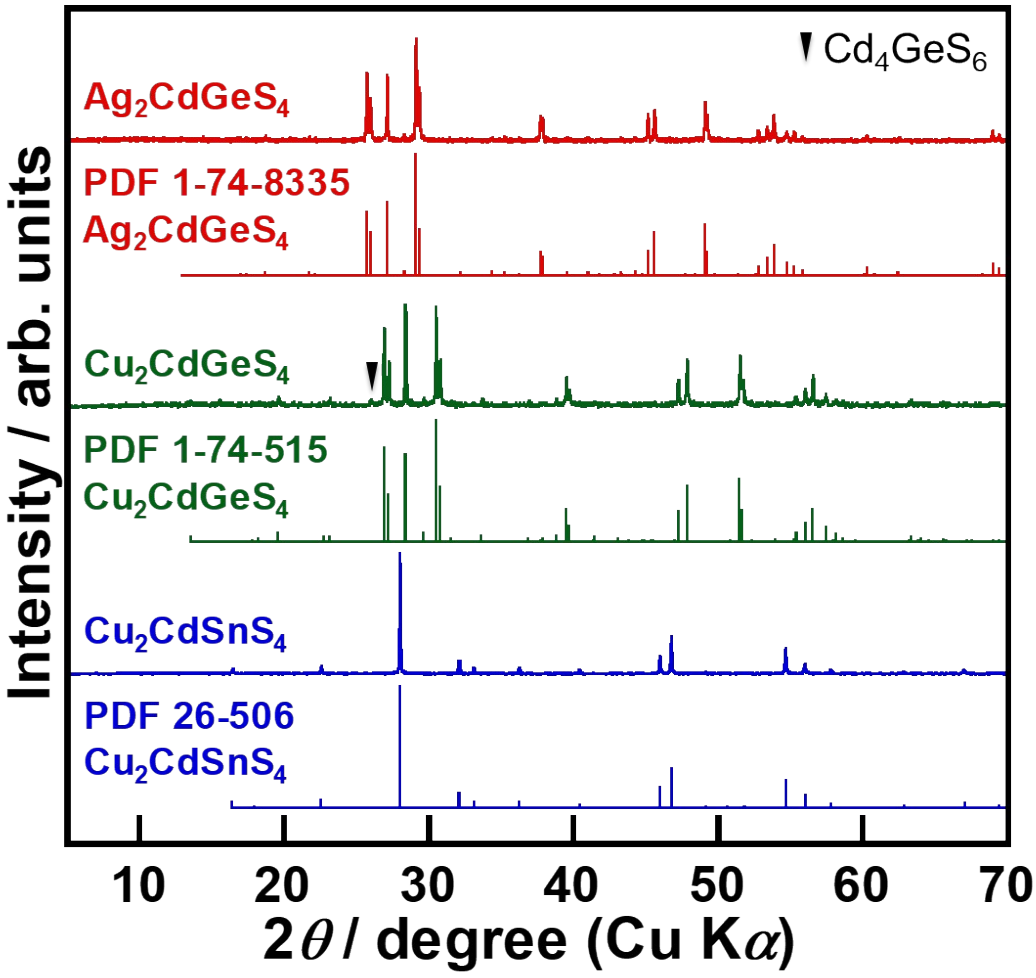


**Figure S1** XRD patterns of $Ag_2CdGeS_4$ and $Cu_2CdMS_4$(M=Ge and Sn) prepared by a solid-state reaction. Patterns due to $Ka_2$ were eliminated.

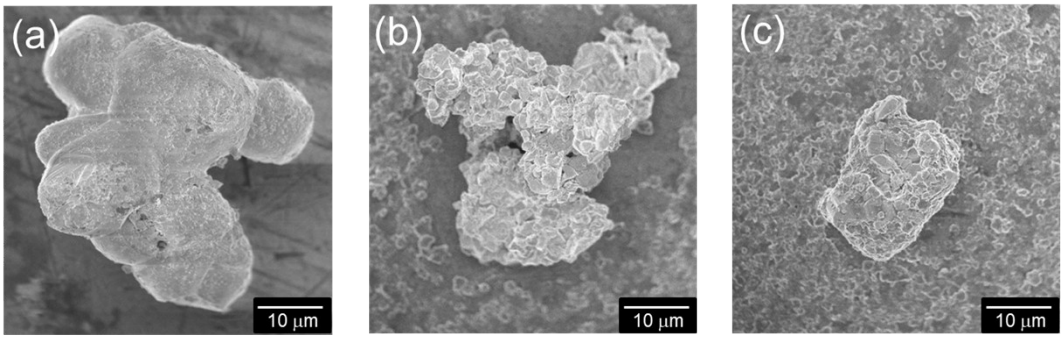


**Figure S2** SEM images of (a) $Ag_2CdGeS_4$, (b) $Cu_2CdGeS_4$ and (c) $Cu_2CdSnS_4$ prepared by a solid-state reaction.

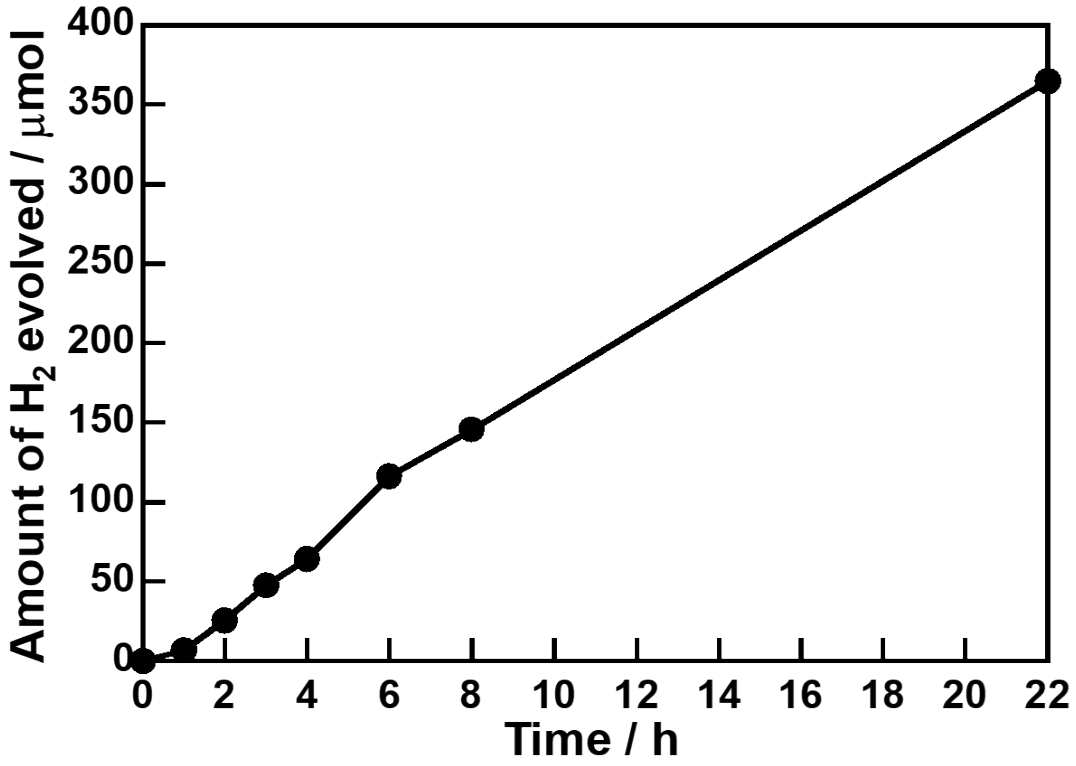


Figure S3 $H_2$ evolution over a Ru-loaded $Cu_2CdSnS_4$ photocatalyst prepared by a solid-state reaction from an aqueous solution containing sacrificial reagents under visible light irradiation. Photocatalyst: 0.3 g, cocatalyst: photodeposition in situ, reactant solution: 0.5 mol $L^{-1}$ $K_2SO_3$ and 0.1 mol $L^{-1}$ $Na_2S$ aqueous solution (120 mL), cell: top-irradiation cell with a Pyrex window, light source: 300 W Xe lamp with a cut-off filter (HOYA: L42).