

Tridecaboron Diphosphide: A New Infrared Light Active Photocatalyst for Efficient CO₂ Photoreduction under Mild Reaction Conditions

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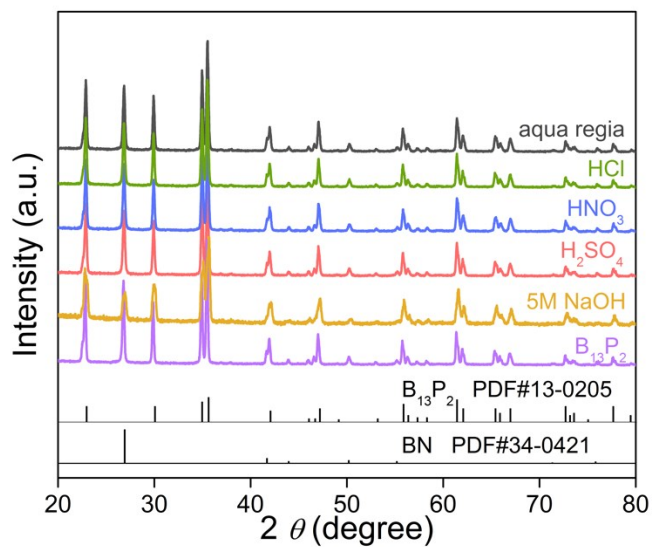


Figure S1. XRD patterns of commercial $B_{13}P_2$ before and after concentrated acid and 5M NaOH solution treatment.

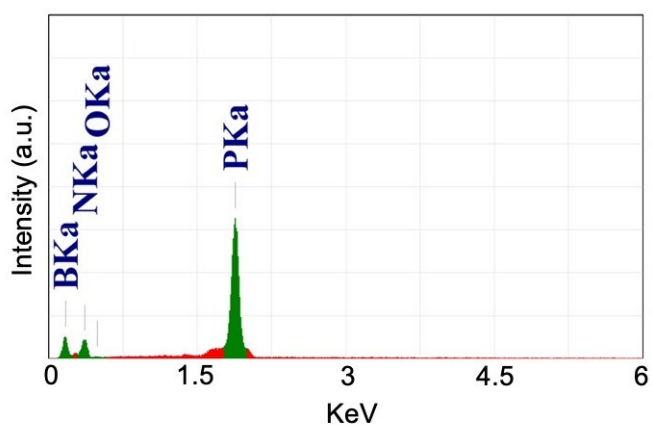


Figure S2. Energy Dispersive Spectrometer (EDS) of commercially available $B_{13}P_2$.

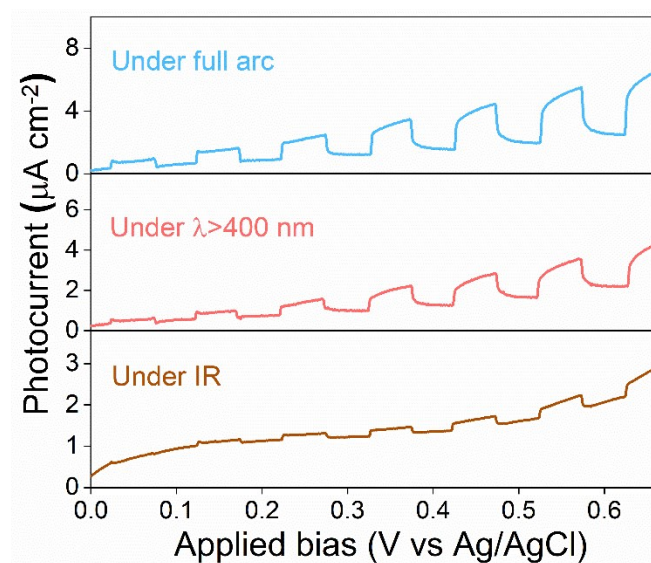


Figure S3. Linear-sweep-voltammetry sweeps for the $B_{13}P_2$ photoanode under full arc, $\lambda > 400\ nm$ and IR light.

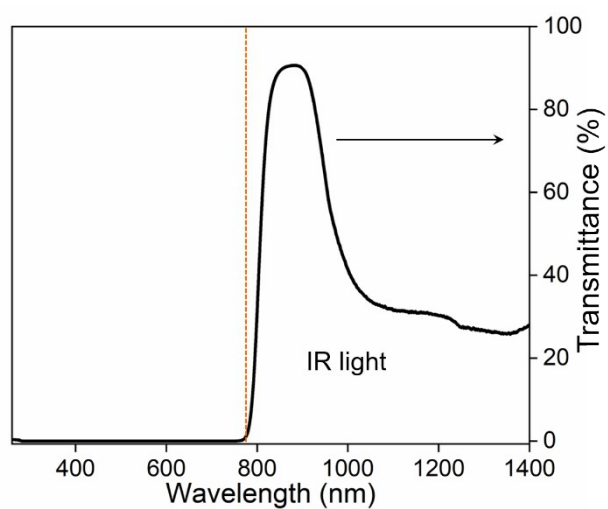


Figure S4. Transmittance spectrum of UV-Vis cutoff filter. It shows that the produced incident light wavelength is $\lambda > 780\ nm$.

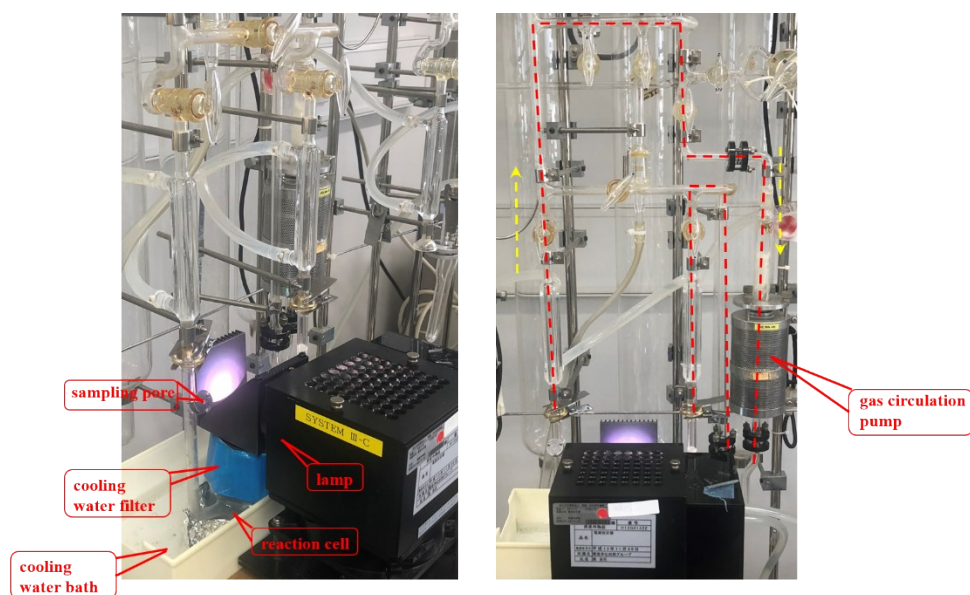


Figure S5. The experimental setup for photocatalytic CO₂ reduction.

Table S1. Comparison of photocatalytic CO₂ reduction performances over different photocatalysts.

photocatalysts	Light source	CO ₂ reduction activity	References
B ₁₃ P ₂	300 W Xe lamp, IR light ($\lambda > 780$ nm)	CO: 0.13 $\mu\text{mol h}^{-1}$	This work
CuS	300 W Xe lamp with AM 1.5 G filter, IR light ($\lambda > 800$ nm)	CO: 0.073 $\mu\text{mol h}^{-1}$	J. Am. Chem. Soc. 2019, 141, 423–430.
Defective WO ₃	40 W silicon nitride lamp, IR light ($\lambda > 800$ nm)	CO: 0.015 $\mu\text{mol h}^{-1}$	Joule 2018, 2, 1004.
UiO-66/CNNS	300 W Xe lamp, visible light (400 nm $< \lambda < 800$ nm)	CO: 0.099 $\mu\text{mol h}^{-1}$	Adv. Funct. Mater. 2015, 25, 5360–5367.
BiOCl	500 W Xe lamp, full arc	CO: 0.101 $\mu\text{mol h}^{-1}$	Nano Research 2015, 8, 821–831.
BiOIO ₃	300 W Xe lamp, full arc	CO: 0.35 $\mu\text{mol h}^{-1}$	Adv. Mater. 2020, 32, 1908350.
Mg-In LDH	200 W Hg-Xe lamp, full arc	CO: 0.4 $\mu\text{mol h}^{-1}$	Angew. Chem. Int. Ed. 2012, 51, 8008–8011.

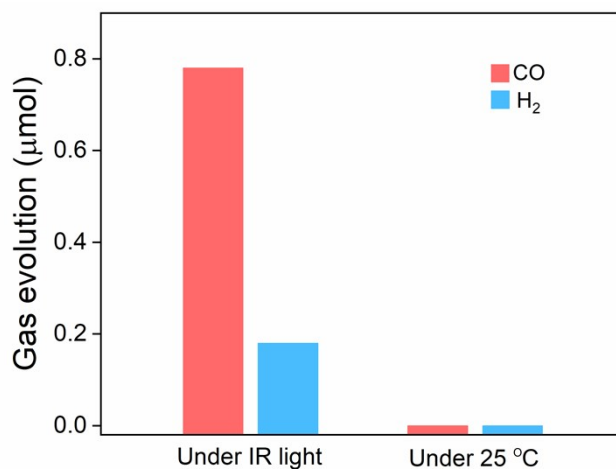


Figure S6. CO and H₂ evolution over B₁₃P₂ under IR light and 25 °C condition without light, respectively. The reaction time is 6 hours and Co(bpy)₃²⁺ is used as cocatalyst.

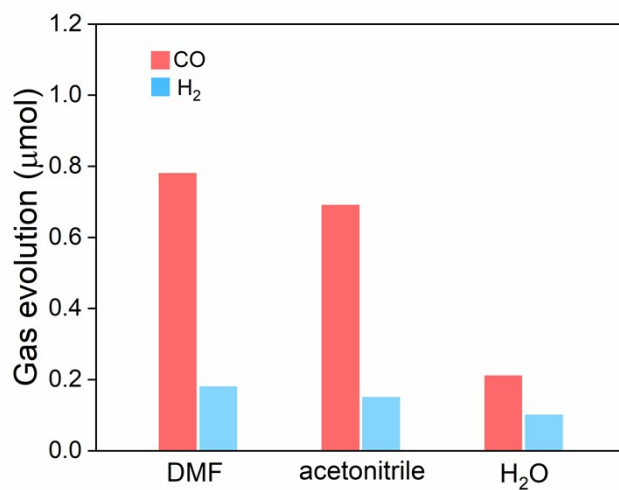


Figure S7. CO and H₂ evolution over B₁₃P₂ under IR light in different solvent in the presence of TEOA as sacrificial agent. The reaction time is 6 hours and Co(bpy)₃²⁺ is used as cocatalyst.

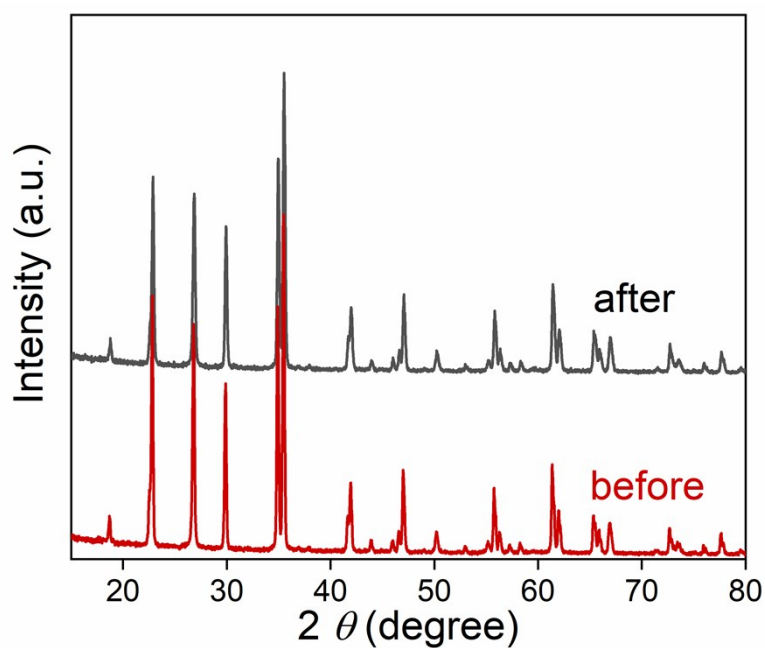


Figure S8. XRD patterns of B₁₃P₂ before and after photocatalytic CO₂ reduction for 6 cycles.

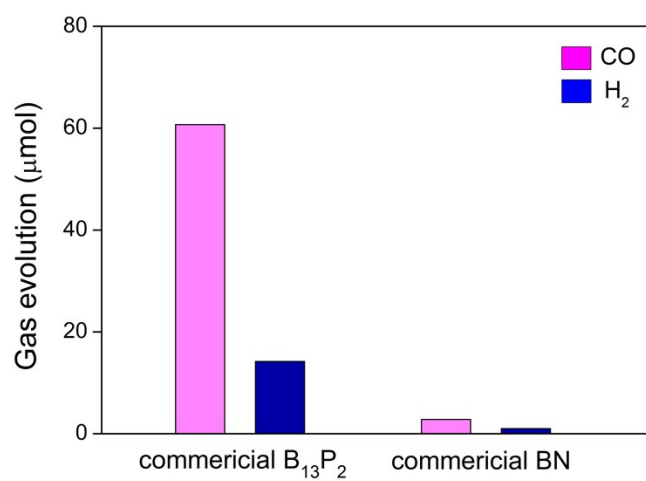


Figure S9. Photocatalytic CO₂ reduction performances over commercial B₁₃P₂ and BN under full arc (UV+ Vis + IR) light irradiation.

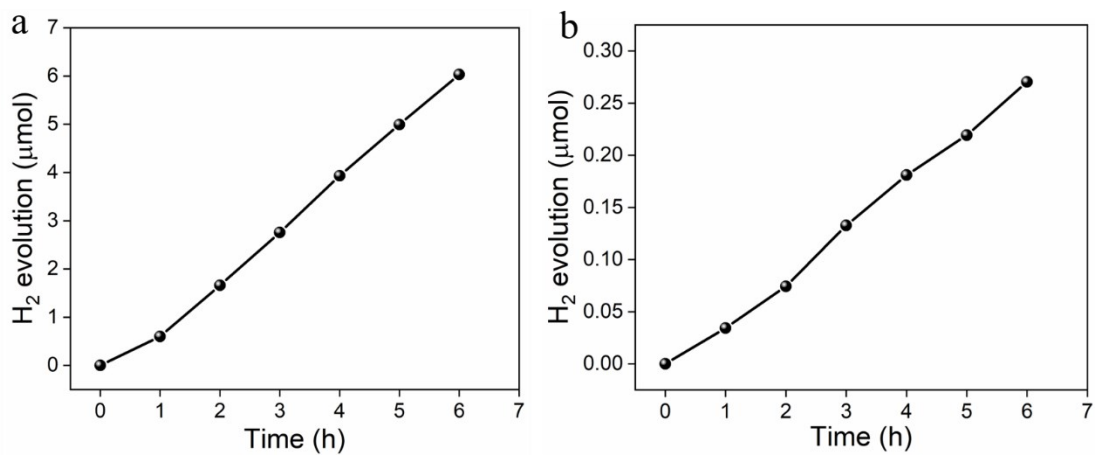


Figure S10. Photocatalytic H₂ evolution performances of B₁₃P₂ under (a) $\lambda > 400$ nm (Vis+ IR) light and (b) IR light.

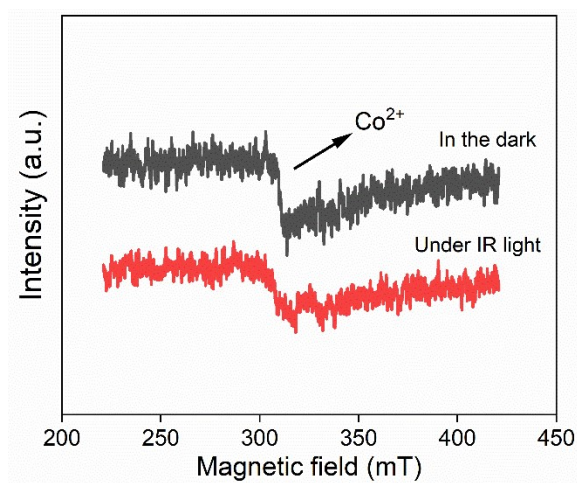


Figure S11. ESR spectra of B₁₃P₂/ Co(bpy)₃²⁺ before and after IR light irradiation.

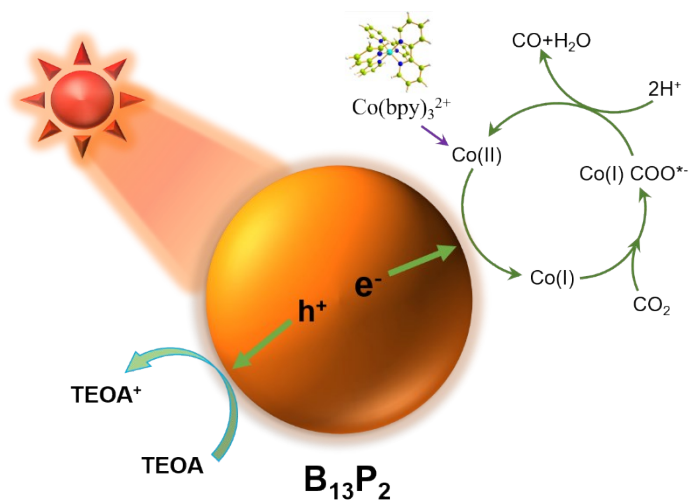


Figure S12. Proposed mechanism of $B_{13}P_2/ Co(bpy)_3^{2+}$ for photocatalytic CO_2 reduction.