

Supporting Information

P25@CoAl-layered double hydroxide heterojunction nanocomposites for CO₂ photocatalytic reduction

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Apparent quantum yield calculations

The apparent quantum yield (AQY) was measured using the same experimental setup, but with band-pass filters of 365 nm for UV light and 480 nm visible light to obtain monochromatic light and the equation as follows:

$$\text{AQY} / \% = \frac{\text{Number of reacted electrons}}{\text{Number of incident photons}} \times 100$$

$$\text{Moles of incident photons (N}_{\text{Einstein}}) = \frac{\text{Number of incident photons (N}_p)}{N_A}$$

Number of incident photons N_p can be calculated by

$$N_p = \frac{\text{Irradiance (E)}}{\text{Photon energy (E}_p)} ; \text{ and Photon energy (E}_p) = \frac{hc}{\lambda}$$

$$E_p = \frac{(6.625 \times 10^{-34} \text{ J} \cdot \text{Sec}) (3 \times 10^{17} \text{ nm Sec}^{-1})}{\lambda \text{ (nm)}} = \frac{19.88 \times 10^{-17}}{\lambda \text{ (nm)}}$$

$$N_p = \frac{E}{E_p} = E \times \lambda \times 5.03 \times 10^{15} (\text{m}^{-2} \text{Sec}^{-1});$$

$$N_{\text{Einstein}} = \frac{N_p}{N_A} = 0.836 \times E \times \lambda \text{ (nm)} \times 10^{-8} (\text{mol} \cdot \text{m}^{-2} \cdot \text{sec}^{-1})$$

$$N_{\text{Einstein}} = 0.836 \times E \times \lambda \text{ (nm)} \times 10^{-2} (\mu\text{mol} \cdot \text{m}^{-2} \cdot \text{sec}^{-1})$$

$$\text{AQY} / \% = \frac{\text{Number of reacted electrons } (\mu\text{mol} \cdot \text{sec}^{-1})}{0.836 \times E \times \lambda \times 10^{-2} (\mu\text{mol} \cdot \text{m}^{-2} \cdot \text{sec}^{-1})} \times 100$$

$$\text{AQY} / \% = \frac{\text{Number of reacted electrons } (\mu\text{mol} \cdot \text{h}^{-1})}{0.836 \times 3600 \times E \times \lambda \times 10^{-2}} \times 100$$

$$\text{AQY} / \% = \frac{\text{Number of reacted electrons } (\mu\text{mol} \cdot \text{h}^{-1})}{30.096 \times E \times \lambda \text{ (nm)}} \times 100$$

where Irradiance (E) = light intensity in reactor × effective light irradiation area. Light intensity within the reactor was measured using a G & R labs intensity meter over the range 190-750 nm.

E is 0.10 W.cm⁻² at 365 nm and 0.12 W.cm⁻² at 475 nm

SPECTRAL DISTRIBUTION

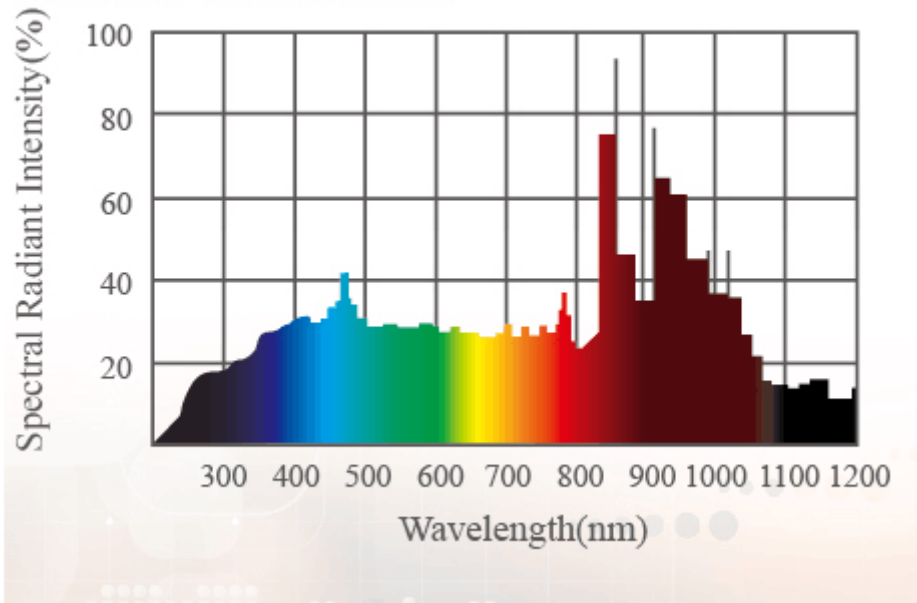


Figure S1. Spectral output of 300 W Xe light source.

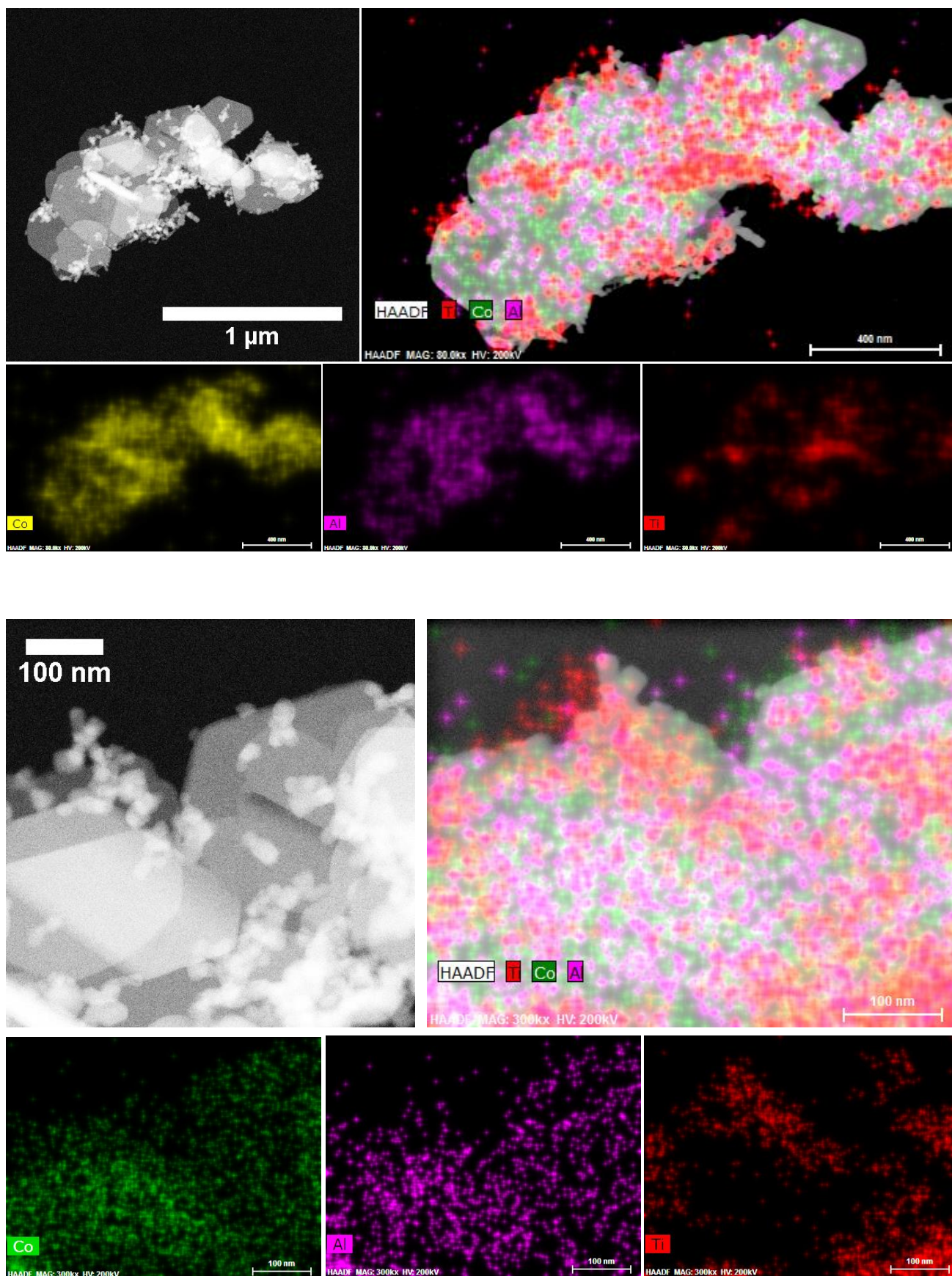


Figure S2. (top) low and (bottom) high resolution TEM images and corresponding EDX element maps of 20 wt% TiO_2 @CoAl-LDH nanocomposite highlighting relatively high and uniform distribution of P25 throughout LDH matrix.

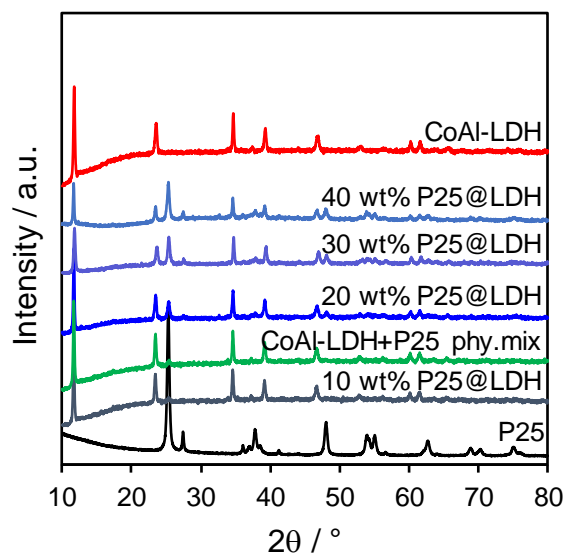


Figure S3. Powder XRD patterns of P25@CoAl-LDH nanocomposites, and reference patterns from P25, CoAl-LDH and a physical mixture of 20wt%P25+CoAl-LDH.

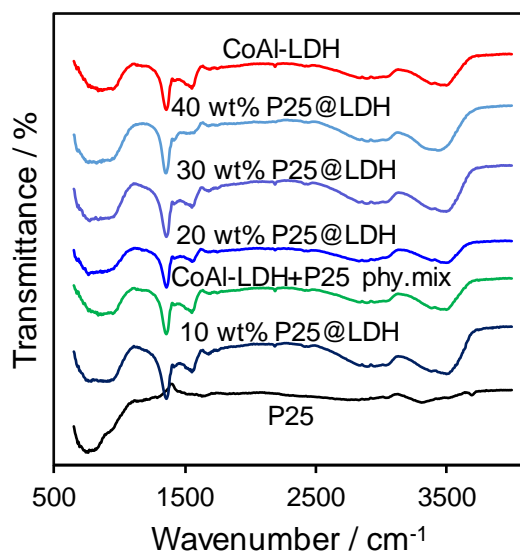


Figure S4. DRIFT spectra of P25@CoAl-LDH nanocomposites, and reference patterns from P25, CoAl-LDH and a physical mixture of 20wt%P25+CoAl-LDH.

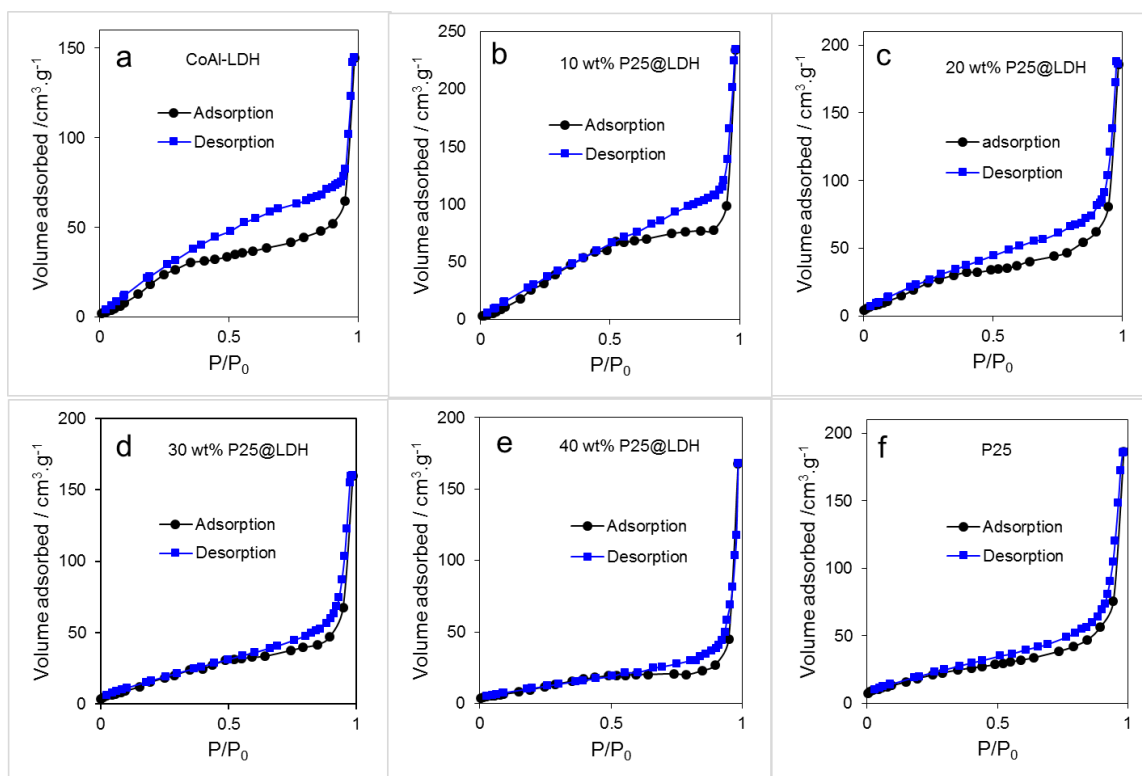


Figure S5. N_2 adsorption-desorption isotherms of CoAl-LDH, P25@CoAl-LDH nanocomposites and P25.

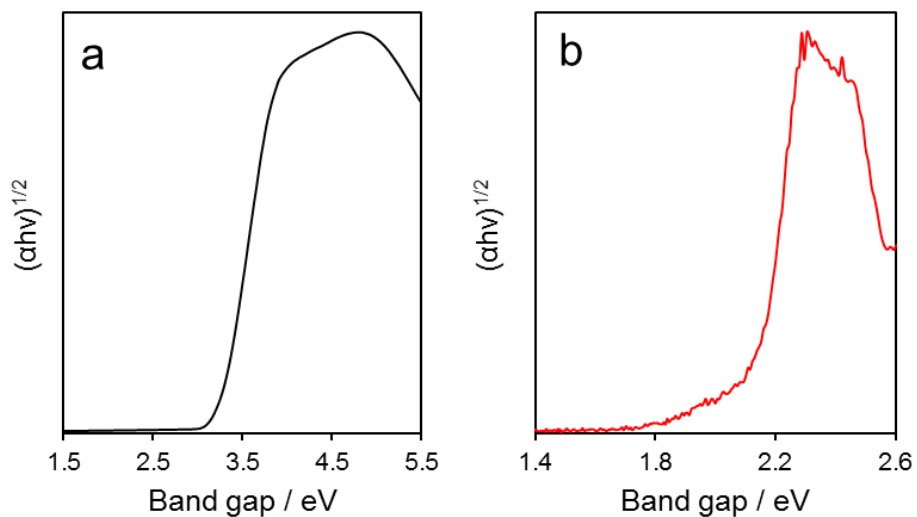


Figure S6. (a) Tauc plot to determine optical band gap of (a) CoAl-LDH and (b) P25 reference materials.

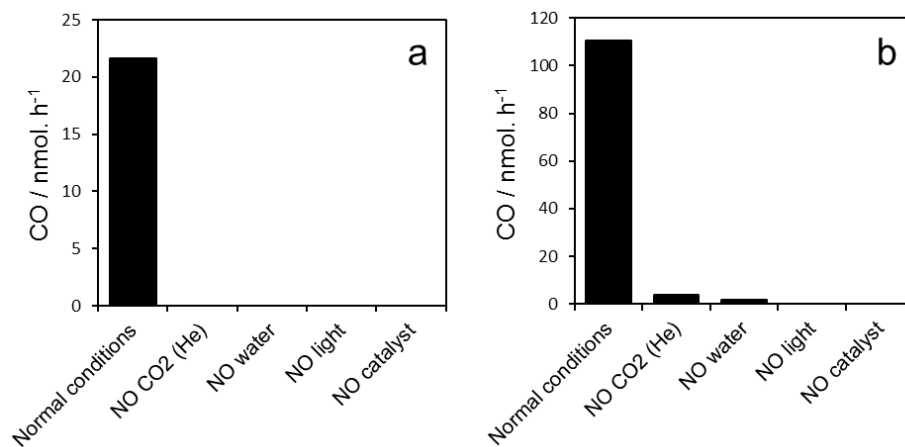


Figure S7. CO productivity during control experiments using (a) P25 and (b) 20 wt% P25@CoAl-LDH.

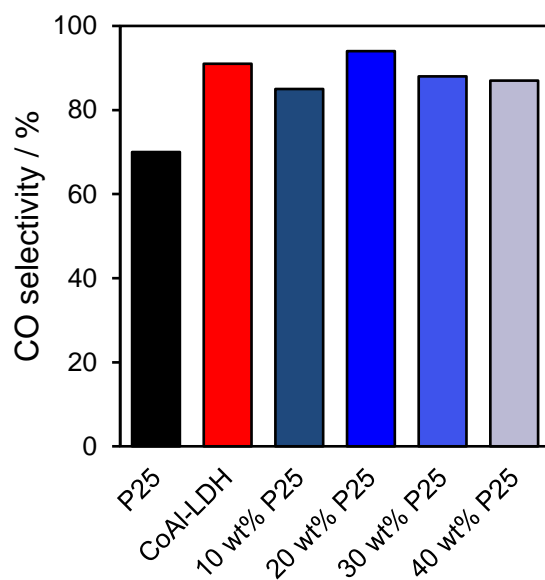


Figure S8. CO selectivity during aqueous phase CO₂ photoreduction over P25 and CoAl-LDH references and P25@CoAl-LDH nanocomposites under UV-visible irradiation.

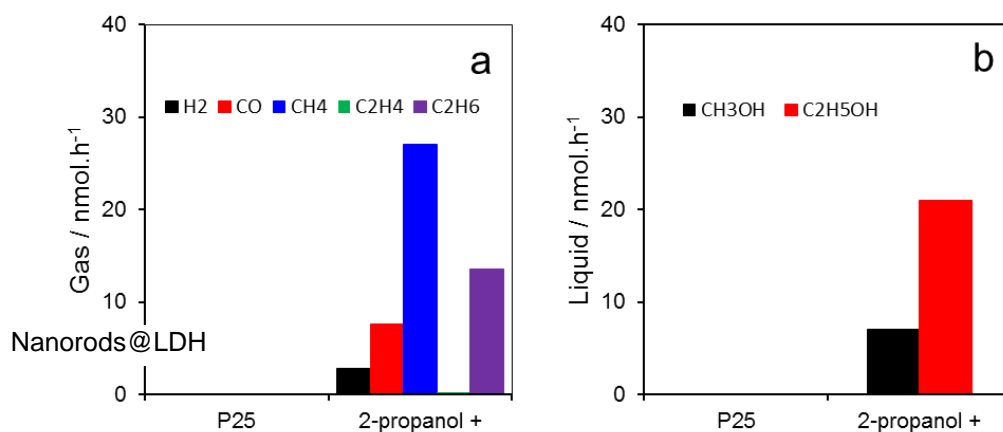


Figure S9. Effect of 2-propanol as a hole scavenger on photocatalytic production of (a) gas and (b) liquid phase carbon containing products during UV-visible irradiation under a He atmosphere.

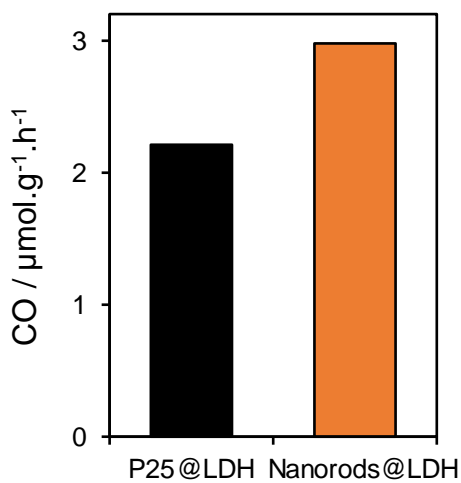


Figure S10. Effect of titania morphology on CO₂ photoreduction over 20 wt% P25@CoAl-LDH and 20 wt% anatase nanorod@CoAl-LDH nanocomposites under UV-visible irradiation. 18 nm long anatase nanorods prepared according to reference 11.

Table S1. Comparative performance of inorganic heterostructures for the photocatalytic reduction of CO₂

| Material | Reaction conditions | Light source | Surface area / m ² .g ⁻¹ | Productivity / μmol.g ⁻¹ .h ⁻¹ | AQE / % | Ref. |
|---|--|-------------------------------------|--|--|--------------------------------------|-----------|
| ZrOCo ^{II} -IrO _x SBA-15 wafer | CO ₂ and water vapor | 355 nm UV light | - | CO=1.74 | 0.001 (355 nm) | [1] |
| Cu ₂ O/RuO _x | 1 bar CO ₂ and 0.7M aqueous Na ₂ SO ₃ | 150 W Xe | - | CO=0.32 | - | [2] |
| Cu ^{II} -grafted Nb ₃ O ₈ nanosheets | CO ₂ and 0.5 M aqueous KHCO ₃ | Hg_Xe | - | CO=0.72 | - | [3] |
| Cu _x O-SrTiO ₃ | CO ₂ and 0.5 M aqueous KHCO ₃ | Hg-Xe | - | CO=0.35 | - | [4] |
| Ce-TiO ₂ /SBA-15 | CO ₂ and water vapor | 450 W Xe (450 mW.cm ⁻²) | 140 | 0.30 (CO=0.25, CH ₄ =0.05) | - | [5] |
| Au@SrTiO ₃ | CO ₂ and water vapor | 300 W Xe | 72 | 0.52 (CO=0.35, CH ₄ =0.17) | - | [6] |
| Cu-PbS-QDs/TiO ₂ | CO ₂ and water | 300 W Xe | - | 1.71 (CO=0.82, CH ₄ =0.58, C ₂ H ₆ =0.31) | - | [7] |
| MgAl-LDO/TiO ₂ | CO ₂ and water vapor <50 °C | 450 W Xe | 175 | CO=1.5 | - | [8] |
| Au@NaTaO ₃ | CO ₂ and water vapor | 200 W Hg-Xe | 21 | 0.20 (CO=0.17, CH ₄ =0.03) | - | [9] |
| In ₂ O _{3-x} (OH) _y Nanocrystal | CO ₂ and water vapor | 1000 W Hortilux Blue metal halide | 159 | CO=1.2 | - | [10] |
| P25@CoAl-LDH | 1 bar CO ₂ and water | 300 W Xe | 57 | CO=2.21 | 0.10 (365 nm) 0.03 (475 nm) | This work |

References

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