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Supporting Information

Hydrophilic Fully Conjugated Covalent Organic Framework for Photocatalytic CO₂ Reduction to CO Nearly 100% by Pure Water

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1. Computational Results

(1) Diagram of building simulation model of LZU1-COF.



(2) Other adsorption structures and adsorption energies of CO_2 and H_2O in LZU1-COF and QL-COF.





3. Supplementary Figures

Figure S1 Schematic and the model reaction equations of the synthesis for LZU1-COF and QL-COF via schiff-base and Doebner reaction, respectively.



Figure S2 XPS spectra of (A) N1s of the LZU1-COF,(B) N1s and (C) O1s of the QL-COF.



Figure S3 Powder X-ray diffraction spectra of the LZU1-COF, QL-COF, Ph(CHO)₃, and Ph(NH₂)₂.



Figure S4 SEM images of (A) LZU1-COF and (B) QL-COF.



Figure S5 TEM images of (A) LZU1-COF and (B) QL-COF.



Figure S6 TGA analysis on the polymers under air, with a ramping rate of 10 °C min.



Figure S7 H_2O contact angles for LZU1-COF and QL-COF.



Figure S8 Adsorption (filled) and desorption (empty) isotherms of CO₂ at 273 k for LZU1-COF and QL-COF.



Figure S9 CO_2 adsorption isotherms of LZU1-COF and QL-COF at 273 K.



Figure S10 Tauc plots together with the bandgaps: (A) LZU1-COF and (B) QL-COF.



Figure S11 Motto-Schottky plots of (A) LZU1-COF and (B) QL-COF. Electrode in 0.2 M Na₂SO₄ (pH=6.8).



Figure S12 GC spectrum of the photocatalytic reaction of CO_2 over QL-COF. Retention time: 1.522 min (O_2), 2.088 min (N_2), 3.259 min (CH_4) and 4.401 min (CO).



Figure S13 ¹³C NMR spectrum for liquid phase of the photocatalytic reaction of ¹³CO₂ over QL-COF.



Figure S14 Average production rates from CO_2 photoreduction over LZU1-COF, QL-COF, TiO₂ and g-C₃N₄ for 5 h.



Figure S15 GC-MS spectrum of ¹³CO generated from the photocatalytic reaction of ¹³CO₂ over QL-COF.



Figure S16 (A) TEM and (B) SEM images of QL-COF-After.



Figure S17 (A) XRD, (B) FT-IR and (C) UV–Vis light absorption spectra of QL-COF and QL-COF-After. (D) UV–Vis light absorption spectra of LZU1-COF and LZU1-COF-After.