Supplementary Information (SI) for EES Catalysis.

Supporting Information

Photo Fluidic Bed Reactor Maximizes Photon Utilization in Heterogeneous Photocatalysis: Theory to Practice

Haojin Wu[1, 2 †], Abdelaziz Gouda[1†*], Shiquan Shan[2], Zhijun Zhou[2], and Geoffrey Ozin[1*]

[1]Solar Fuels Cluster, Department of Chemistry, University of Toronto, 80 Saint George Street, Toronto, ON, M5S 3H6, Canada

[2]State Key Laboratory of Clean Energy Utilization, Zhejiang University, Hangzhou 310027, China

† Authors contributed equally to this work.

***Corresponding authors**

E-mail: Abdelaziz.gouda@utoronto.ca

E-mail: g.ozin@utoronto.ca

The calculation of photon to yield efficiency:

In this study, the photon to yield efficiency is calculated by the ratio of the number of CO molecules generated to the number of photons absorbed [1]:

$$Photon\ to\ yield = \frac{produced\ CO\ molecules\ per\ unit\ time}{absorbed\ photon\ numbers\ per\ unit\ time}$$

The produced CO molecules is calculated from the CO generate rate. The absorbed photon numbers is estimated from the spectrum dispersion of the xenon lamp and the absorption rate of the carbon particles. The absorbed photon numbers N_{photo} can be expressed as:

$$N_{photo} = \int_{300}^{2400} \frac{I * Spec_{Xe} * A_{carbon} * S}{\frac{hc}{\lambda} * N_A}$$

Where, the I is the light intensity; $Spec_{Xe}$ is the xenon lamp spectral intensity distribution (Fig S5); A_{carbon} is the carbon absorptivity; S is the illumination area; h is the Planck constant; c is the speed of light; λ is the wavelength; N_A is the Avogadro constant.

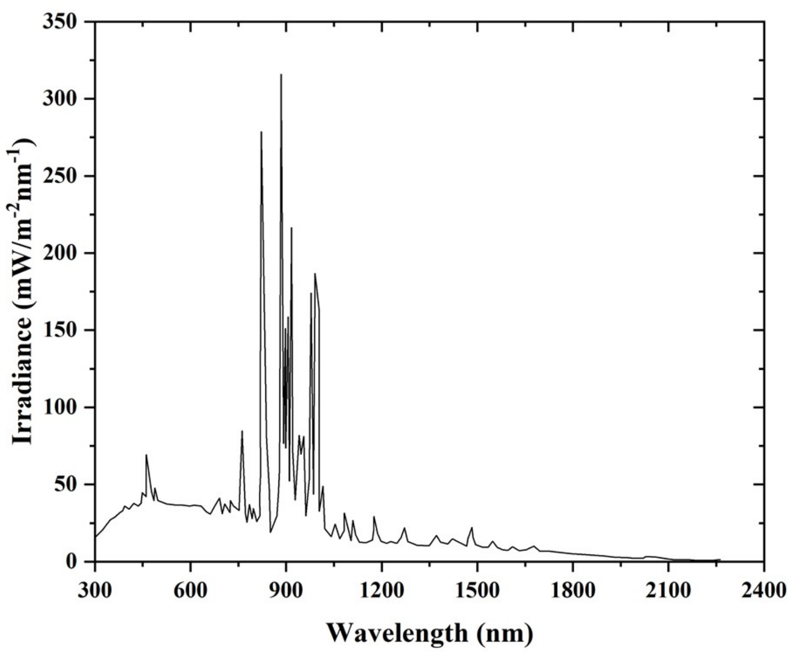

Fig S1. Spectral intensity distribution of the 300 W Xenon lamp.

Table S1. Photon to yield efficiency.

Catalyst and reaction	Photon to yield efficiency	reference
Solar reverse Boudourd reaction in PFBR	0.04% (48.41 W/m^2)	This work
Solar reverse Boudourd reaction in Fixed bed	0.02% (48.41 W/m^2)	This work
$Ni_{12}P_5$ for reverse water gas shift (RWGS)	0.06 %	[1]
Cu–Fe/ TiO_2–SiO_2 for CO_2 photocatalytic to methane	0.05 %	[2]
TiO_2 nanotubes for CO_2 photocatalytic to methane	0.06 %	[3]

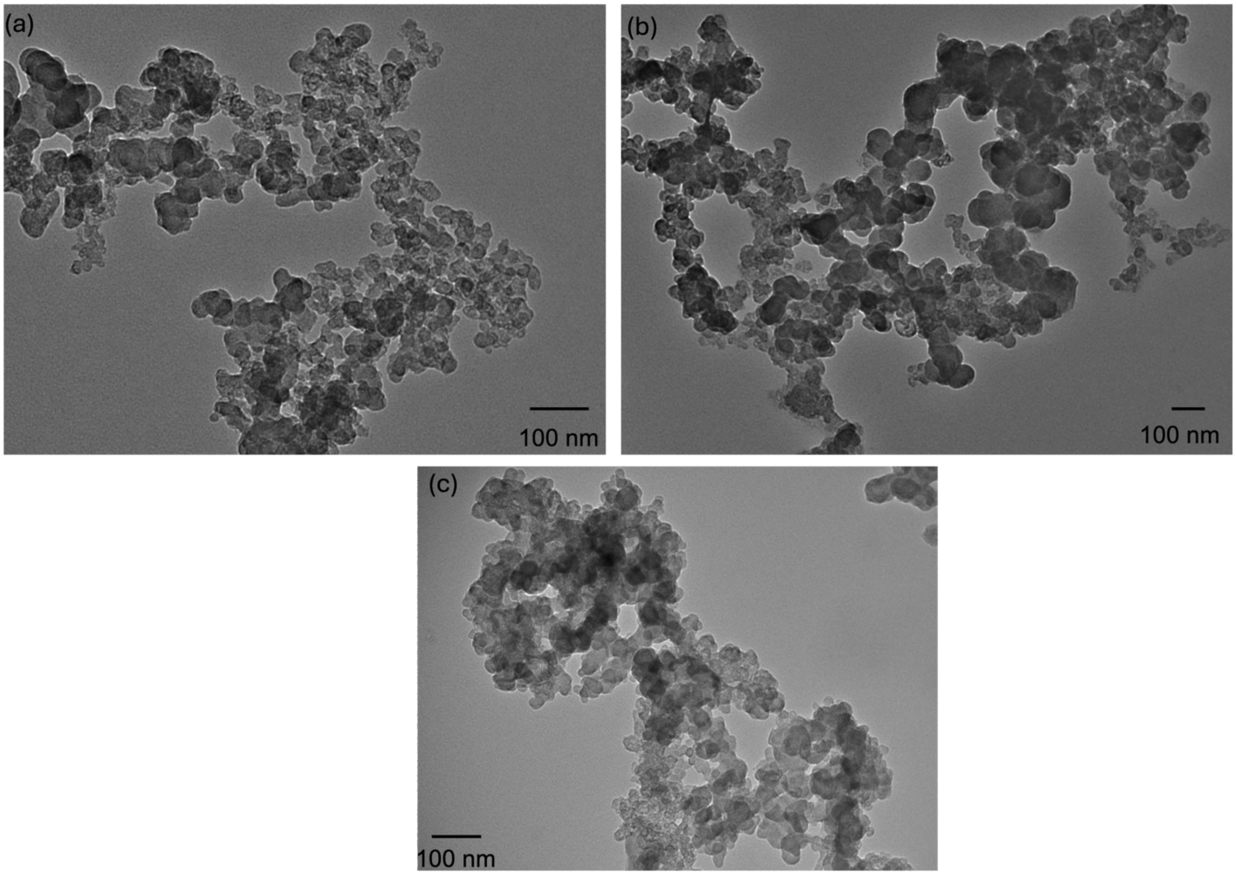

Fig. S2. TEM images of (a) pristine carbon before the reaction. (b) Carbon after reaction in fixed bed reactor (FBR). (c) Carbon after reaction in Photo fluidized bed reactor (PFBR).

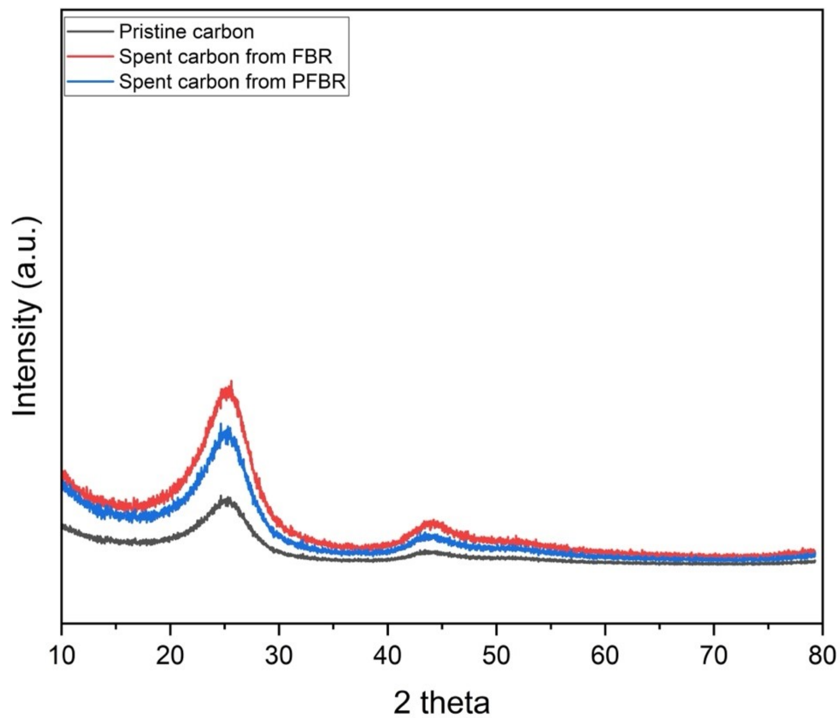

Fig S3. PXRD pattern of carbon samples before and after reaction in FBR and PFBR.

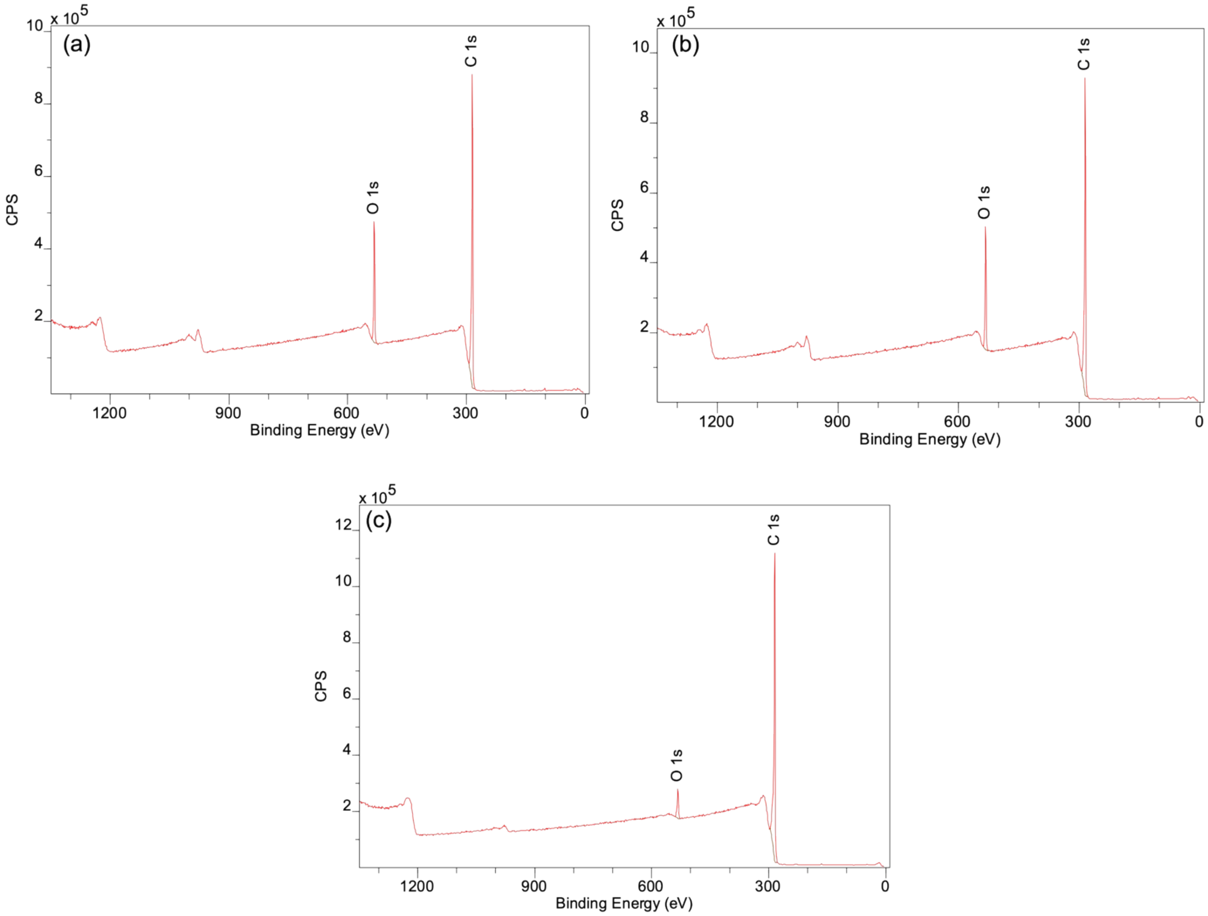

Fig S4. XPS survey scan of (a) pristine carbon. (b) spent carbon from FBR. (c) spent carbon from PFBR.

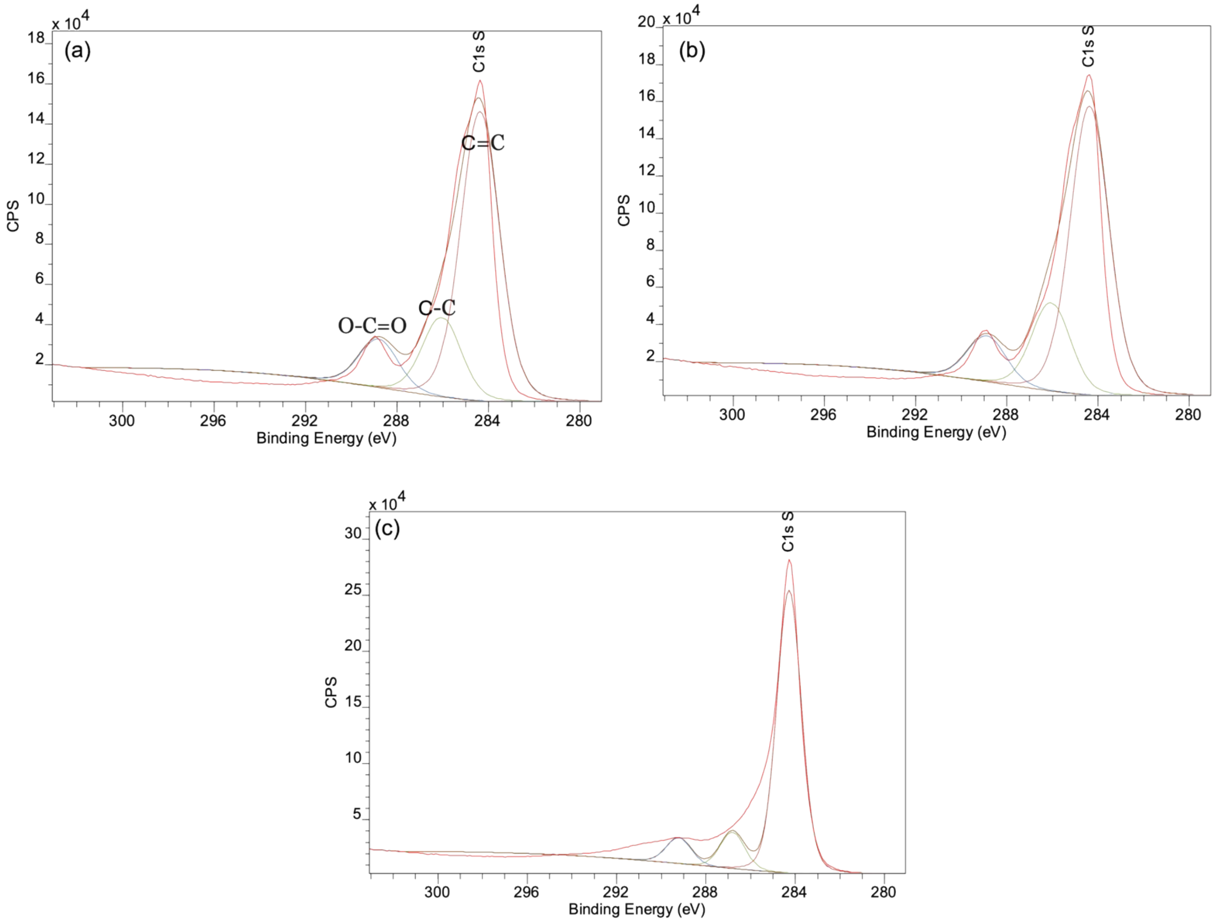

Fig S5. C1s high-resolution XPS spectrum of (a) pristine carbon. (b) spent carbon from FBR. (c) spent carbon from PFBR.

Table S2. Identification and quantification of elements from XPS survey scans for carbon before and after the reaction from FBR and PFBR.

Group Name	**Binding Energy (eV)**	**Identification**	**Atomic %**		
			Pristine carbon	Spent carbon from FBR	Spent carbon from PFBR
C - 1s	285.10	element total	88.85	88.81	96.70
O - 1s	533.10	element total	11.15	11.19	3.30

Reference:

1. Xu, Y.-F., et al., *High-performance light-driven heterogeneous CO2 catalysis with near-unity selectivity on metal phosphides.* Nature Communications, 2020. **11**(1): p. 5149.
2. Nguyen, T.-V. and J.C.S. Wu, *Photoreduction of CO2 to fuels under sunlight using optical-fiber reactor.* Solar Energy Materials and Solar Cells, 2008. **92**(8): p. 864-872.
3. Cortes, M.A.L.R.M., et al., *Formal quantum efficiencies for the photocatalytic reduction of CO2 in a gas phase batch reactor.* Catalysis Today, 2019. **326**: p. 75-81.