

Supplementary Information

Gas phase photocatalytic CO₂ reduction, “A brief overview for benchmarking”

Shahzad Ali^{1†}, Monica Claire Flores^{1†}, Abdul Razzaq^{2†}, Saurav Sorcar¹, Chaitanya B. Hiragond¹, Hye Rim Kim¹, Young Ho Park¹, Yunju Hwang¹, Hong Soo Kim¹, Hwapyong Kim¹, Eun Hee Gong¹, Junho Lee¹, Dongyun Kim¹, and Su-Il In^{1*}

¹Department of Energy Science & Engineering, DGIST, 333 Techno Jungang-daero, Hyeonpung-eup, Dalseong-gun, Daegu 42988, Republic of Korea

²Department of Chemical Engineering, COMSATS University Islamabad, Lahore Campus, 1.5 KM Defence Road, Off Raiwind Road, Lahore, 54000, Pakistan

* Correspondence: insuil@dgist.ac.kr; Tel.: +82-053-785-6417

† These authors contributed equally to this work

Calculation of AQY:

Photocatalytic reaction with Pt/TiO₂ mesoporous photocatalyst from [1]:

Main product: **CH₄**

Reactor type: Batch reactor (quartz tubular reactor)

Product yield: 5.7 $\mu\text{mol g}_{\text{cat}}^{-1}$ after 120 mins

Apparent Light input (H): 348 W/m²

Area of irradiation (A): computed from tubular reactor dimensions

(length: 28.0 cm $\times$ diameter: 3.0 cm) A = 0.0084 m²

Band gap: 3.18 eV

The number of reacted electrons is computed by

$$\text{number of reacted electrons} = \left[\frac{\text{mole of product}}{\text{produced in time, t}} \right] \times \left[\frac{\text{number of electrons required to produce}}{1 \text{ mol of product}} \right] \times N_A$$

Since $\text{CO}_2 + 8\text{H}^+ + 8\text{e}^- \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$, there are 8 electrons required to produce 1 mol of CH₄ product

$$\begin{aligned} \text{number of reacted electrons} &= \left[\frac{5.7 \times 10^{-6} \text{ mol}}{2} \right] \times [8] \times 6.022 \times 10^{23} \text{ per mol} \\ \text{number of reacted electrons} &= 1.37 \times 10^{19} \end{aligned}$$

The number of incident photons is computed by

$$\text{effective number of incident photons} = \frac{\text{light absorbed by the photocatalyst}}{\text{average photon energy}} \times t$$

Wherein light absorbed by the photocatalyst and average photon energy is found to be

$$\text{light absorbed by the photocatalyst} = H \times A = 348 \frac{\text{W}}{\text{m}^2} \times 0.0084 \text{ m}^2 = 2.92 \text{ W}$$

$$\text{average photon energy} = \frac{hc}{\lambda}$$

Where λ is the average wavelength of the absorption range of the photocatalyst. We first computed the maximum wavelength from the band gap by using the formula:

$$\lambda_{\text{max}} = \frac{hc}{E_g} = \frac{(6.626 \times 10^{-34} \text{ J}\cdot\text{s}) \times (3 \times 10^8 \text{ m/s})}{3.18 \text{ eV}} \times \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} \times 10^9 = 390 \text{ nm}$$

Therefore, the average wavelength would be

$$\lambda = \frac{\lambda_{\text{min}} + \lambda_{\text{max}}}{2} = \frac{250 + 390}{2} = 320 \text{ nm}$$

The average photon energy is then computed to be

$$\text{average photon energy} = \frac{(6.626 \times 10^{-34}) \times (3 \times 10^8)}{320 \times 10^{-9} \text{ m}} = 6.21 \times 10^{-19} \text{ J}$$

$$\text{number of incident photons} = \frac{2.92 \text{ W}}{4.91 \times 10^{-19} \text{ J}} \times \frac{3600 \text{ s}}{\text{hr}}$$

$$\text{number of incident photons} = 1.69 \times 10^{22}$$

AQY computation:

$$\text{AQY (\%)} = \frac{\text{number of reacted electrons}}{\text{effective number of incident photons}} \times 100\%$$

$$\text{AQY (\%)} = \frac{1.37 \times 10^{19}}{1.69 \times 10^{22}} \times 100\% = 0.081\%$$

Table S1: Computation of AQY performance of photocatalysts by In et al.

Photocatalyst	Product	Product Yield ($\mu\text{mol/g/h}$)	Light input (W/m^2)	Area of irradiation (m^2)	Band gap (eV)	Wavelength		Ave. λ (nm)	No. of reacted electrons	Average photon energy (J)	No. of incident photons	AQY (%)
<i>Degussa P25</i> [2]	CH₄	0.021	1200	0.00071	-	250	365	308	1.01×10^{17}	6.46×10^{-19}	4.74×10^{19}	0.0021
<i>CZTS</i> [3]	CH₄	0.082	1000	0.00071	1.5	250	828.3	539	3.95×10^{17}	3.69×10^{-19}	6.93×10^{21}	0.0057
<i>CZTS-ZnO</i> [4]	CH₄	0.095	1000	0.00041	1.74	250	714	482	4.58×10^{17}	4.12×10^{-19}	3.58×10^{21}	0.0128
<i>Cu_xO-TiO₂</i> [5]	CH₄	0.152	1000	0.00071	3.15	250	394.4	322	7.32×10^{17}	6.17×10^{-19}	4.14×10^{21}	0.0177
<i>Pt-X-RT</i> [6]	CH₄	1.13	1000	0.00071	2.85	250	435.9	343	5.44×10^{18}	5.8×10^{-19}	4.41×10^{21}	0.1234
<i>C,N-TNT06</i> [7]	CH₄	9.75	1000	0.00071	2.8	250	443.7	347	4.7×10^{19}	5.73×10^{-19}	4.46×10^{21}	1.0532
<i>Pt-XG/RBT</i> [8]	CH₄	37	1000	0.00049	2.41	250	515.5	383	1.78×10^{20}	5.19×10^{-19}	3.4×10^{21}	5.2479
	C₂H₆	11	1000	0.00049	2.41	250	515.5	383	9.27×10^{19}	5.19×10^{-19}	3.4×10^{21}	2.7303
<i>Pt-BT-X</i> [9]	CH₄	80.35	1000	0.00049	2.73	250	455.1	353	3.87×10^{20}	5.63×10^{-19}	3.13×10^{21}	12.36
<i>Cu_x%-Pt_y%-BT</i> [10]	CH₄	500	1000	0.00049	2.85	250	435.9	343	2.41×10^{21}	5.8×10^{-19}	3.04×10^{21}	79.14
	C₂H₆	25	1000	0.00049	2.85	250	435.9	343	2.11×10^{20}	5.8×10^{-19}	3.04×10^{21}	6.92

Table S2: Computation of AQY performance of photocatalysts from other research works

Photocatalyst	Product	Product Yield	Light input	Area of irradiation	Band gap	Wavelength		Ave. λ	No. of reacted electrons	Average photon energy (J)	No. of incident photons	AQY (%)
		($\mu\text{mol/g/h}$)	(W/m^2)	(m^2)	(eV)	λ_{min}	λ_{max}	(nm)				
$\text{Cd}_{1-x}\text{Zn}_x\text{S}$ ¹	CH₄	0.22	2850	0.00091	2.33	400	510	455	1.06×10^{18}	4.37×10^{-19}	2.14×10^{22}	0.0049
[11]	CO	2.9	2850	0.00091	2.33	400	510	455	3.49×10^{18}	4.37×10^{-19}	2.14×10^{22}	0.0163
Co-ZIF-9/TiO_2 ¹	CO	17.58	4940	0.00081	-	200	900	550	2.12×10^{19}	3.61×10^{-19}	3.98×10^{22}	0.053
[12]												
Pt/TiO_2 ¹	CH₄	2.85	348	0.0084	3.18	250	391	320	1.37×10^{19}	6.21×10^{-19}	1.69×10^{22}	0.081 ³
[1]												
$\text{In}_2\text{O}_3\text{-C}_3\text{N}_4$ ¹	CH₄	7.991	12000	0.00063	2.8	250	444	347	3.85×10^{19}	5.73×10^{-19}	4.71×10^{21}	0.082 ³
[13]												
$\text{TiO}_{2-x}/\text{CoO}_x$ ¹	CH₄	0.0903	200	0.00139	-	<i>ave</i>	365	365	4.35×10^{17}	5.45×10^{-19}	1.84×10^{21}	0.0237
[14]	CO	1.2473	200	0.00139	-	<i>ave</i>	365	365	1.50×10^{18}	5.45×10^{-19}	1.84×10^{21}	0.0817
$\text{HCP-TiO}_2\text{-FG}$ ¹	CH₄	27.62	4330	0.00031	2.34	420	531	475	1.33×10^{20}	4.18×10^{-19}	1.17×10^{22}	1.14
[15]	CO	21.63	4330	0.00031	2.34	420	531	475	2.61×10^{19}	4.18×10^{-19}	1.17×10^{22}	0.2227
$\text{Pd}_x\text{Cu}_{1-x}\text{-TiO}_2$ ¹	CH₄	19.6	20	0.0064	-	250	400	325	9.44×10^{19}	6.12×10^{-19}	7.53×10^{20}	12.53 ³
[16]												
In/TiO_2 ¹	CH₄	244	400	0.0012	3.2	250	388	319	1.18×10^{21}	6.23×10^{-19}	2.77×10^{21}	42.39 ³
[17]	CO	81	400	0.0012	3.2	250	388	319	9.76×10^{19}	6.23×10^{-19}	2.77×10^{21}	3.52 ³
ZnV_2O_4 ¹	CH₃OH	100	200	0.0012	2.1	250	592	421	3.61×10^{20}	4.72×10^{-19}	1.83×10^{21}	19.75 ³
[18]	CO	485	200	0.0012	2.1	250	592	421	5.84×10^{20}	4.72×10^{-19}	1.83×10^{21}	31.92 ³
Cu/GO-2 ²	CH₃OH	2.94	1000	0.00442	2.51–3.09	402	495	449	1.06×10^{19}	4.43×10^{-19}	3.59×10^{22}	0.0296
[19]	CH₃CHO	3.88	1000	0.00442	2.51–3.09	402	495	449	2.34×10^{19}	4.43×10^{-19}	3.59×10^{22}	0.065

¹ Batch reactor

² Continuous flow reactor

³ 250 nm was used as the minimum wavelength (λ_{min}) if the light wavelength range was not specified by the reference paper.

**All other AQYs not included here have been computed by the respective authors of the reference paper.

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