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Supporting Information

Selective photo-reduction of CO_2 to methanol using Cu doped 1D-Bi_2S_3/rGO nanocomposite under visible light irradiation

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Content

1. The EDX analysis of (2%) Cu-BSNC/rGO [(2 wt%) Cu doped Bi_2S_3/rGO]

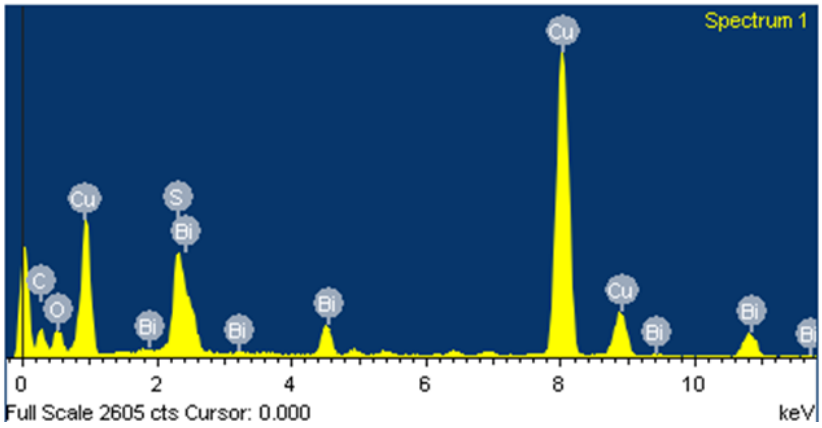


Fig. S1 EDX analysis of (2%) Cu-BSNC/rGO [(2 wt%) Cu doped Bi_2S_3/rGO]

2. GCMS analysis image of BSNC [Bi_2S_3 rod-shaped nanocapsules]

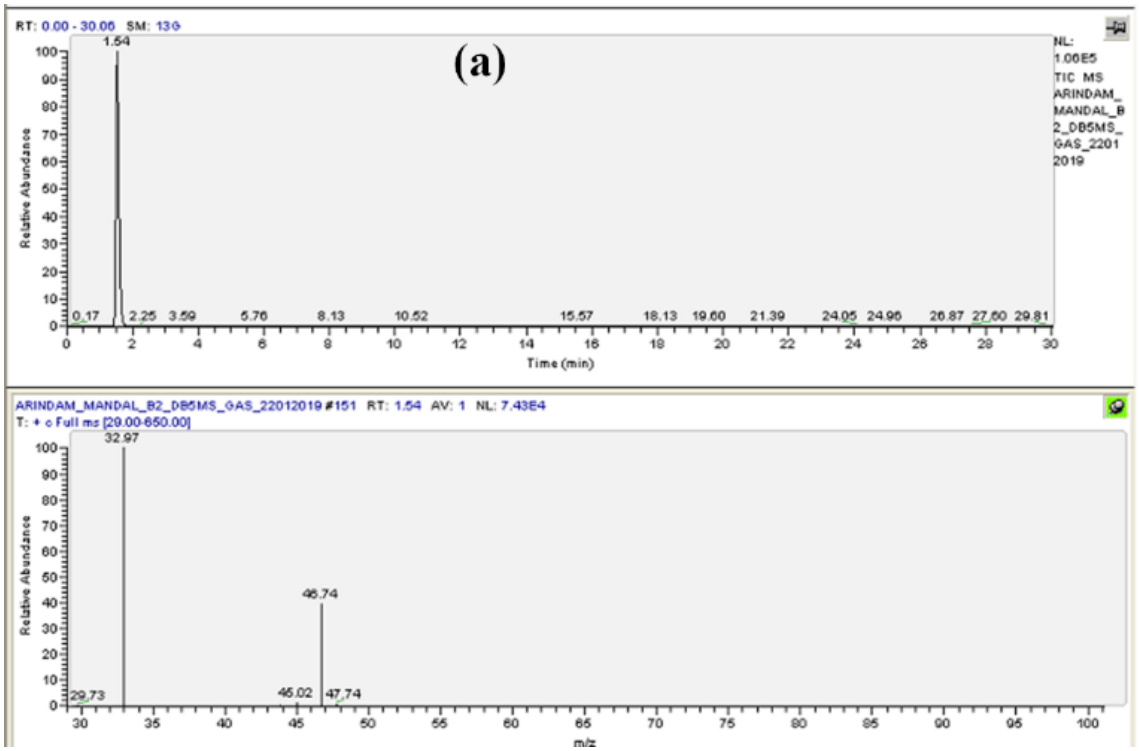


Fig. S2(a) GCMS analysis image of BSNC [Bi_2S_3 rod-shaped nanocapsules].

3. GCMS analysis image of BSNC/rGO [Bi_2S_3/rGO]

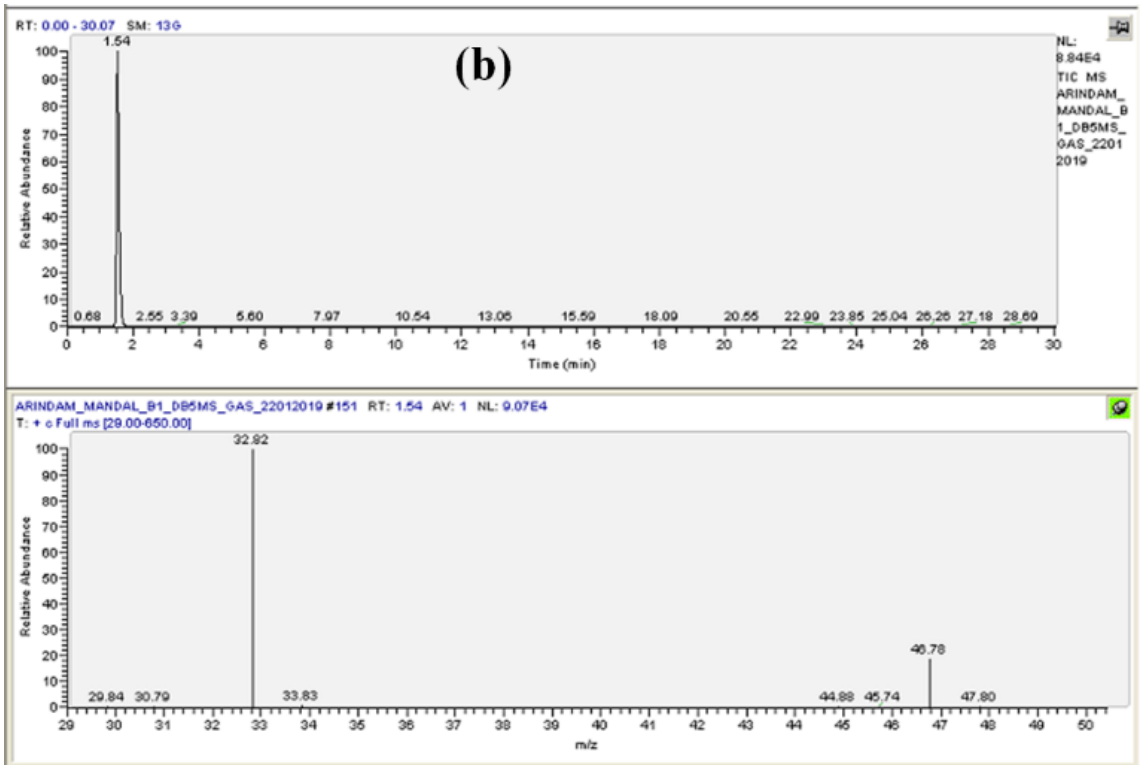
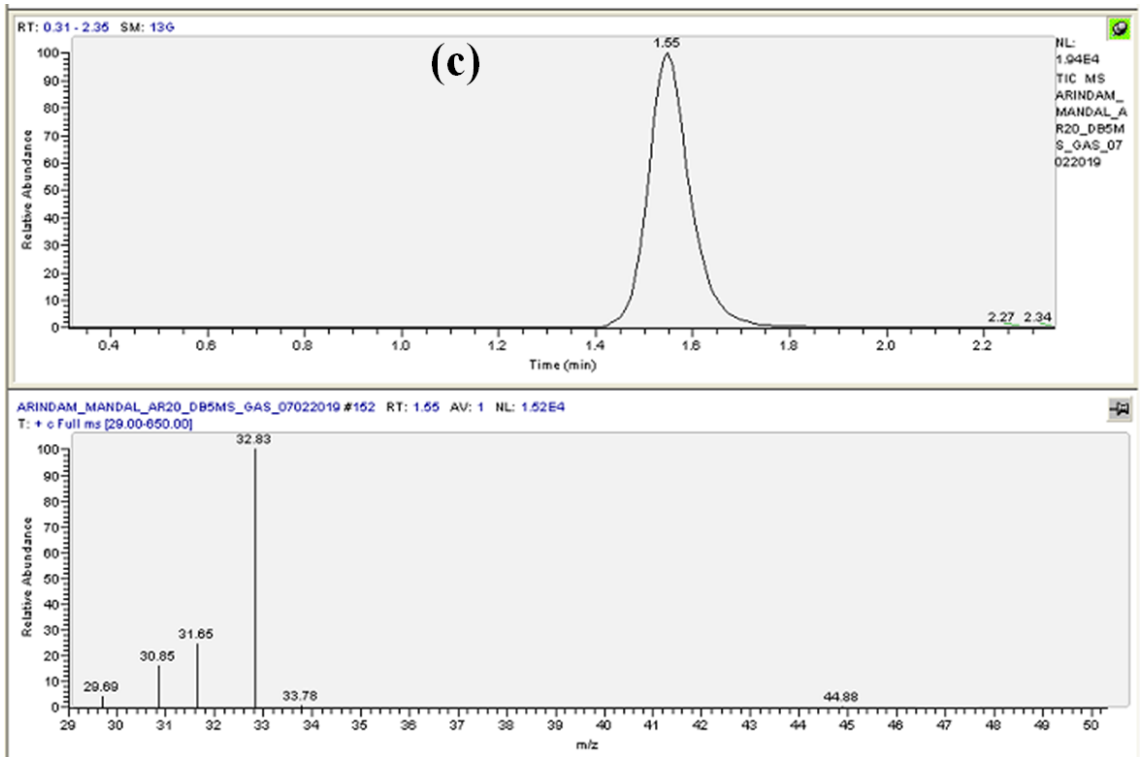


Fig. S2(b) GCMS analysis image of BSNC/rGO [Bi_2S_3/rGO]

4. GCMS analysis images of (1%) Cu-BSNC/rGO [(1 wt%)Cu doped Bi_2S_3/rGO]



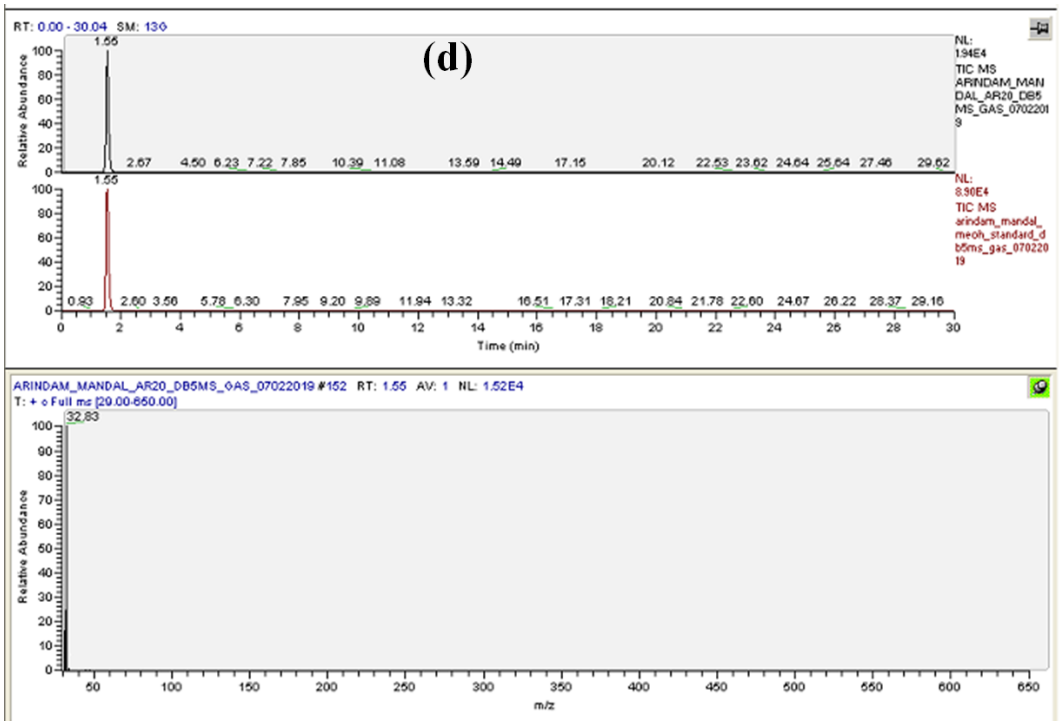


Fig. S2(c) & (d) GCMS analysis images of (1%) Cu-BSNC/rGO [(1 wt%)Cu doped Bi_2S_3/rGO]

5. <u>GCMS analysis image of (1 wt%) Cu-BSNC</u>

The photocatalytic activity study of (1%) Cu-BSNC is also performed for comparison purpose; GCMS analysis detects both methanol, formic acid as photocatalytic CO_2 reduced products in liquid phase. In this study Methanol and formic acid formation are clearly identified by the value of m/z=32.76 & m/z=46.78, respectively, at retention time 1.50 min.

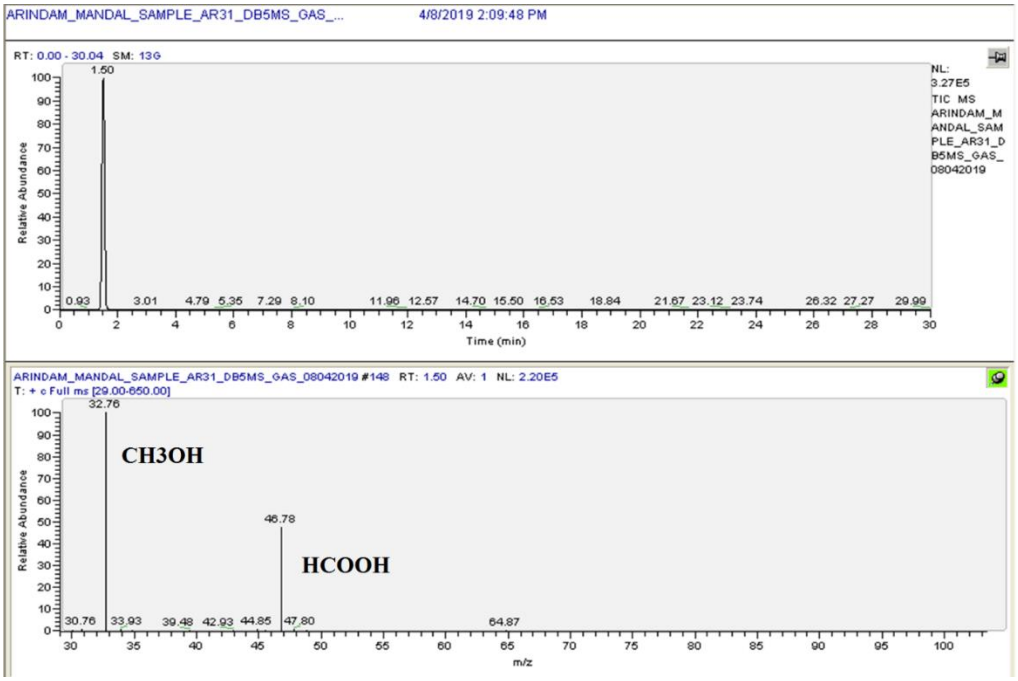


Fig. S2 (e) GCMS analysis image of (1%) Cu-BSNC.

6. Apparent Quantum Yield (AQY) calculation for 1% Cu-BSNC/rGO (1%Cu doped Bi_2S_3/rGO):

Apparent quantum yield (AQY) is defined as the ratio of number of reacted electrons to the number of incident photons. [Reference (59) -J. Am. Chem. Soc. 2020,142, 4862−4871]

$$AQY = \frac{\text{Number of reacted electrons}}{\text{Number of incident photons}} \times 100 \quad \ldots\ldots (1)$$

As given in equation (1), during the photocatalytic reduction of CO_2, stoichiometrically 6 electrons are required to produce one molecule of CH_3OH.

$$CO_2 + 6H^+ + 6e^- \longrightarrow CH_3OH + H_2O \quad \ldots\ldots (2)$$

Therefore, number of reacted electrons can be calculated by directly multiplying 6 with mole of CH_3OH produced during the photocatalytic reaction.

Number of reacted electrons= $[CH_3OH] \times 6 \times N_A$ ..... (3)

where $[CH_3OH]$ = mole of CH_3OH produced in time (t) & N_A = Avogadro's number (6.022×10^{23} mol^{-1})

$[CH_3OH]$ = 215.174 µmol g^{-1} h^{-1} at 420 nm, where t = 10h.

Therefore,

Number of reacted electrons = $215.174\times10^{-6} \times 6 \times 6.022\times10^{23} = 7.775\times10^{20}$

$$\text{Now, Number of photons} = \frac{\text{Light absorbed by the photocatalyst}}{\text{The average photon energy}} \times t \quad \ldots\ldots (4)$$

where; t = time taken for the reaction

Light absorbed by the photocatalyst = E × A

E= Input from the source of the light = 37.5 mW/cm^2 = 375 W/m^2

A= 16.81 cm^2

Light absorbed by the photocatalyst= 375 × 0.001681= 0.630375 J/sec

The average photon energy = hc/λ

h =Planck's Constant= 6.626×10^{-34} J.sec; c = velocity of light =3×10^8 m/sec

λ = Maximum emission wavelength for the spectrum of the source = 420 nm = 420×10^{-9} m

The average photon energy (hc/λ) = 4.7329×10^{-19}

Therefore,

Number of incident photons = $(0.630375/4.7329\times10^{-19})\times36000$ [using equation (4)]

= 4.795×10^{22} photons

AQY= $(7.775\times10^{20}/ 4.795\times10^{22}) \times100$ = **1.62%**