Supplementary material

Visible-Light-Driven CO_2 Reduction into Methanol Utilizing Sol-Gel-Prepared CeO_2-Coupled Bi_2O_3 Nanocomposite Heterojunctions

Mohamed Mokhtar Mohamed Mostafa [1,*], Ahmed Shawky [2,*], Sharif Fakhruz Zaman [3], Katabathini Narasimharao [1], Mohamed Abdel Salam [1], Abdulmohsen Ali Alshehri [1], Nezar H. Khdary [4], Sulaiman Al-Faifi [1] and Abhishek Dutta Chowdhury [5]

[1] Chemistry Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia
[2] Nanomaterials and Nanotechnology Department, Advanced Materials Institute, Central Metallurgical R&D Institute (CMRDI), P.O. Box 87, Cairo 11421, Egypt
[3] Chemical and Materials Engineering Department, King Abdulaziz University, Jeddah 21589, Saudi Arabia
[4] King Abdulaziz City for Science and Technology, Riyadh 11442, Saudi Arabia
[5] College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, China
* Correspondence: mmoustafa@kau.edu.sa (M.M.M.M.); phyashawky@gmail.com (A.S.)

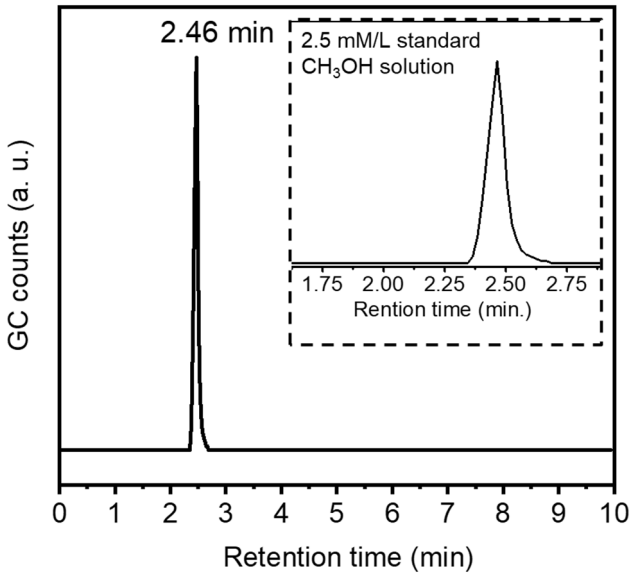

Figure S1. Gas chromatograph of standard 2.5 mM/L CH_3OH solution showing a single peak at 2.46 min retention. The spectra is used as a reference to compare the selective photoreduction of CO_2 over the prepared Bi_2O_3/CeO_2 nanocomposites in the main manuscript.

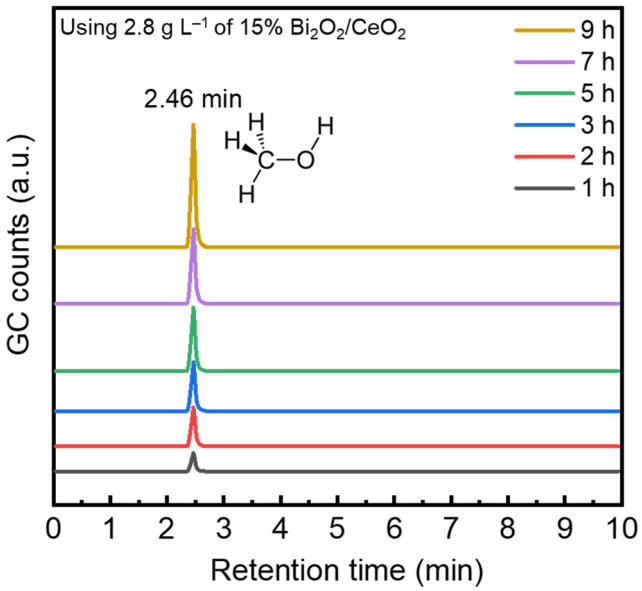

Figure S2. Gas chromatograph of the produced product over the optimized dose 2.8 g/L of 15% Bi_2O_3/CeO_2 showing the accumulated production of CH_3OH over time of irradiation.

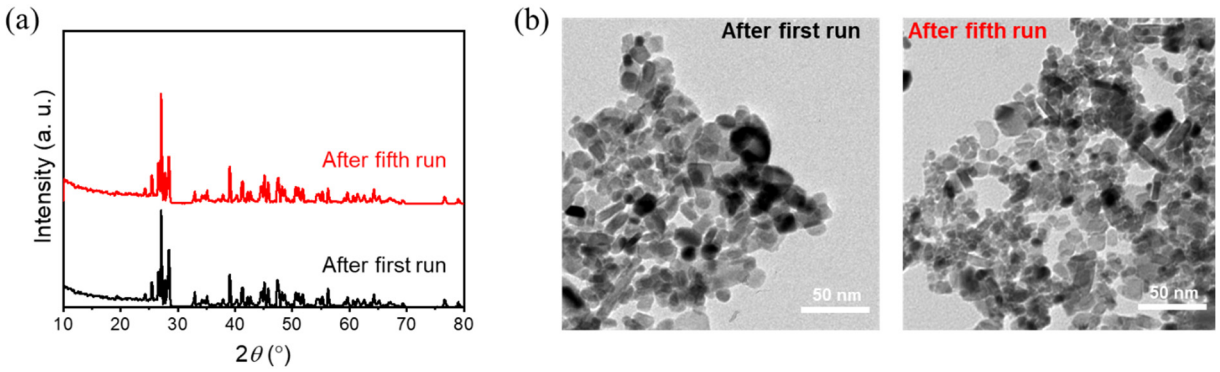

Figure S3. XRD patterns (a) and TEM images (b) of the spent nanocomposite after the first and the fifth runs displaying no substantial change in the crystalline phase or morphological structure after recycling for five times.

The conduction band (CB) and valence band (VB) edges can be calculated through eq's (1) and (2)

$E_{CB} = \chi - E_e - 0.5E_g$ (1) $E_{VB} = E_{CB} + E_g$ (2)

Where E_{VB} and E_{CB} are the VB and CB potentials, respectively. Moreover, E_e is the energy of free electrons vs. hydrogen (4.5 eV). Finally, χ is the electronegativity of semiconductor and it was calculated by the following equation:

$$\chi = [x(A)^a x(B)^b x(C)^c]^{1/(a+b+c)} \quad (3)$$

In which a, b, and c are the number of atoms in the compounds. For example, in the case of La:$NaTaO_3$, the calculation procedure is as follows:

χ for CeO_2 is 5.56 ()

$E_{CB} = 5.56 - 4.5 - (0.5 \times 2.93)$ is -0.405 eV

$E_{VB} = -0.405 + 2.93$ equals 2.525 eV

χ calculation for Bi_2O_3

For Bi: 4.69 eV and For O: 7.54 eV

$\chi\, Bi_2O_3 = (4.69 \times 4.69 \times 7.54 \times 7.54 \times 7.54)^{1/5} = 6.2357$ eV

$E_{CB} = 6.2357 - 4.5 - (0.5 \times 2.4)$ is 0.535 eV

$E_{VB} = 0.535 + 2.4$ equals 2.93 eV