Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Ni Supported $CdIn_2S_4$ Spongy-like Spheres: A Noble Metal Free High-Performance Sunlight Driven Photocatalyst for Hydrogen Production

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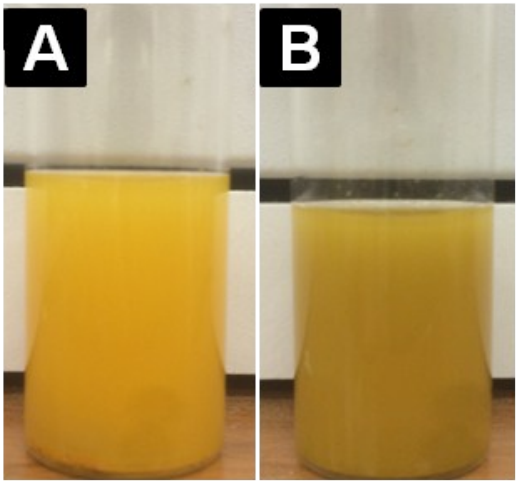

Figure S1 Color of the $CdIn_2S_4$ solution **(A)** before and **(B)** after photo-deposition of Ni.

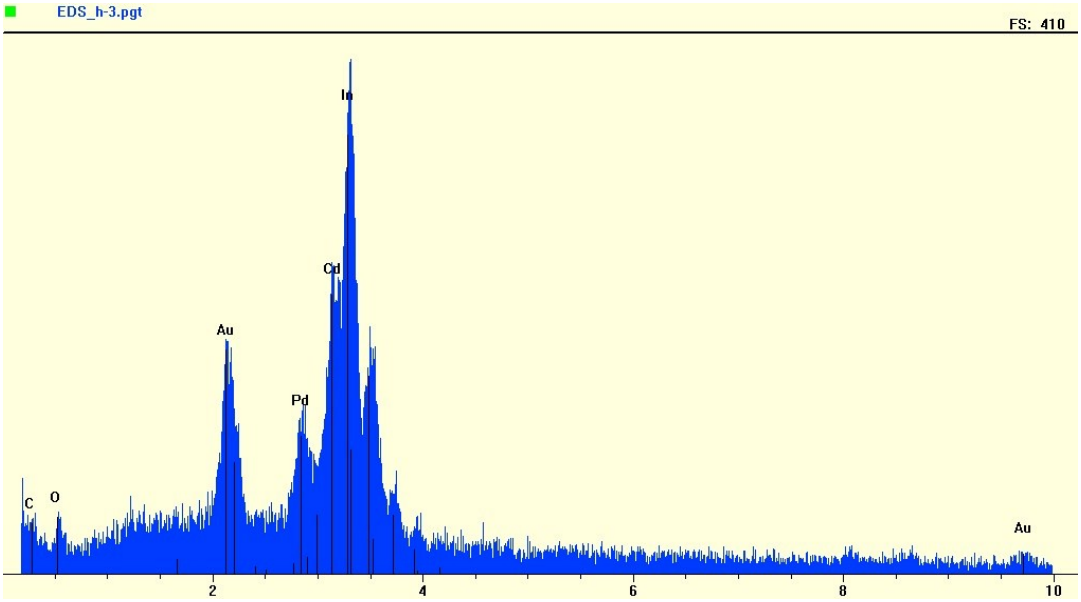

Figure S2: EDX spectrum of $CdIn_2O_4$ spongy-like spheres.

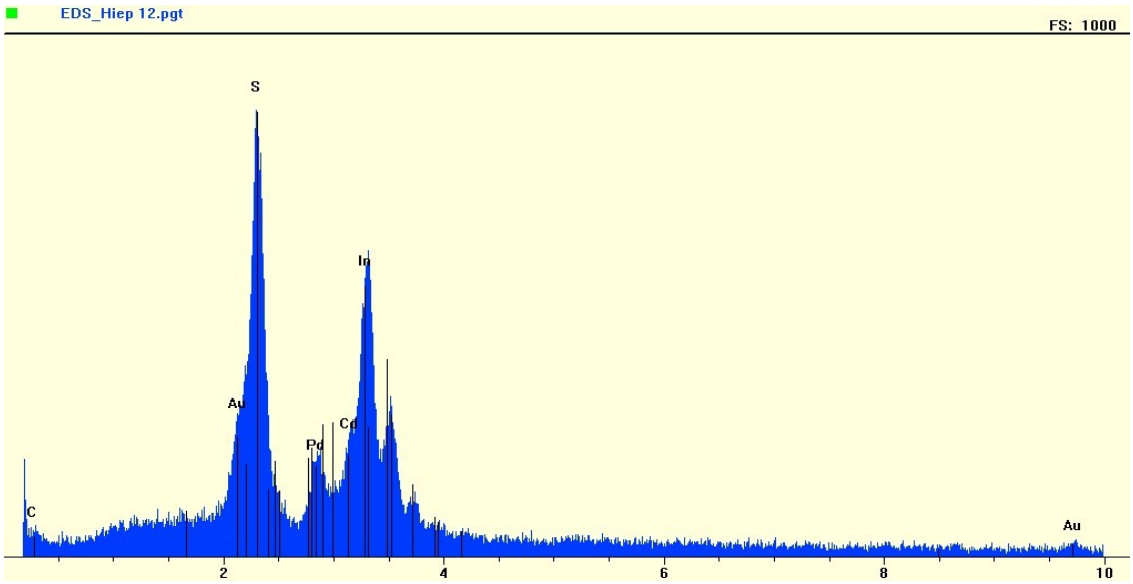

Figure S3 EDX spectrum of $CdIn_2S_4$ spongy-like spheres.

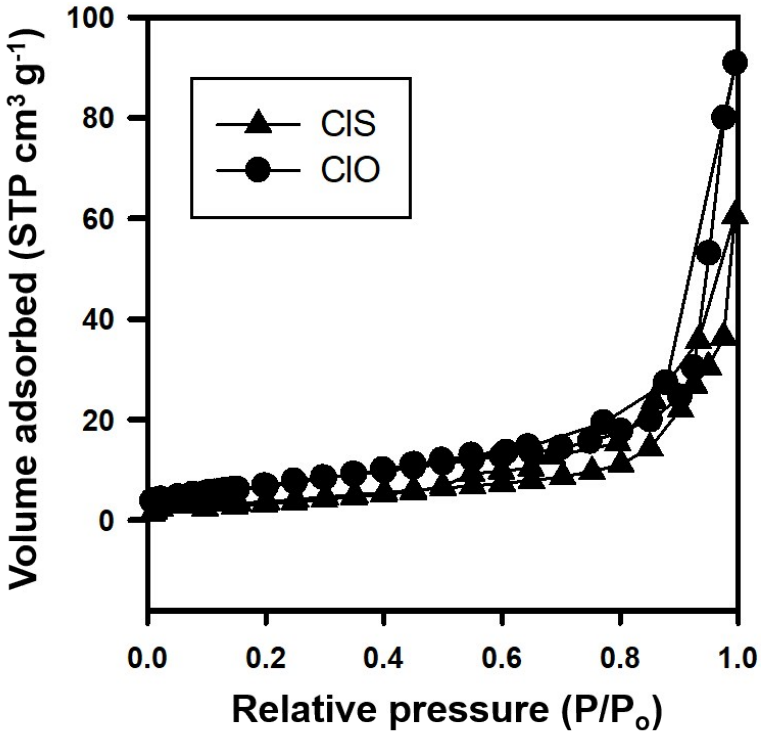

Figure S4 N_2 adsorption-desorption isotherm curves of $CdIn_2O_4$ and $CdIn_2S_4$ spongy-like spheres.

S1. Band edge potential calculations

The band edge position of the material was calculated using the well known and standard empirical equations that widely reported in the literature.[1-4]

$$E_{CB} = X - E^e - 0.5E_g \quad (1)$$

$$E_{VB} = E_{CB} + E_g \quad (2)$$

Where, the X is the electronegativity of the semiconductor which is $CdIn_2S_4$ and it was calculated using the following formula,

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

Where A, B and C are the constituted elements, i.e. Cd, In and S respectively; and a, b, c are the respective number of atoms in the composition, which is 1, 2 and 4, respectively (as in $CdIn_2S_4$).

x(A) can be calculated as follows,

x(A) = [Ionization energy of the element + electron affinity of the element]/2

x(Cd) = [8.9938 + 0.725]/2 = 4.8594

x(In) = [5.78636 + 0.3]/2 = 3.0432

x(S) = [10.36001 + 2.07]/2 = 6.215

Substitute above values in Eqn. (3) as follows,

$X(CdIn_2S_4) = [4.\ 8594 \times (3.0432)^2 \times (6.215)^4]^{1/7}$

$X(CdIn_2S_4) = [67144.15]^{1/7} = 4.89$

$E_{CB} = 4.89 - 4.5 - (0.5 \times 2.23) = -0.73$ eV

$E_{VB} = -0.725 + 2.23 = +1.50$ eV

S2. Apparent quantum efficiency of H_2 evolution

The apparent quantum efficiency (AQE) of the photocatalyst depends on various parameters that include the measurement methods, reaction conditions, amount of photocatalyst taken, wavelength taken for the estimations, etc.[5-7]

The details of AQE calculation as follows;

The evolved H_2 molecules at the end of 3 h, for 15 mg of photocatalyst at the irradiation wavelength of 420 nm was found to be 0.383 μmol and accordingly, AQE was estimated using the following formula and it was found to be 3.35%.

AQE (%) = [Number of reacted electrons or holes]/[number of incident photons] x 100 = [2 x number of H_2 molecules evolved]/[number of incident photons] x 100

References

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