Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Information

Fabrication of $CuInS_2$ photoelectrode using a facile single-step electrodeposition with controlled calcination atmosphere

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1. SEM images of N_2 calcined $CuInS_2$ and H_2/N_2 calcined $CuInS_2$

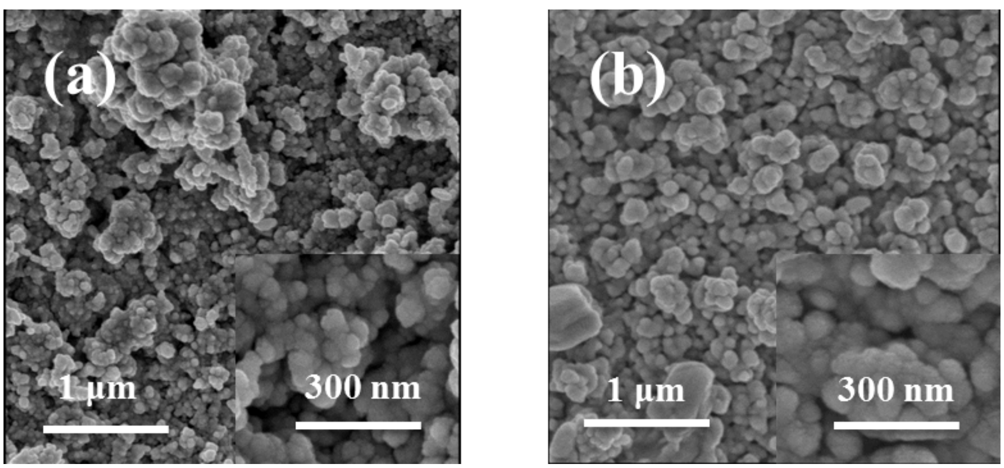

Figure S1 Surface morphology of $CuInS_2$ thin films on FTO substrate using 30 min deposition time calcinated under (a) N_2; (b) 92% N_2 + 8% H_2 for 1 h at 500 °C, and the precursor molar ratio for electrodeposition precursor is $CuCl_3$: $InCl_3$: $Na_2S_2O_3$ = 1: 1 : 10.

The analyses of slopes and flatband potential based on Mott-Schottky plots are performed as below:

$$\text{slope} = \frac{d\left(\frac{1}{C^2}\right)}{dV} = \frac{2}{e_0 \varepsilon \varepsilon_0 N_d A^2}, \ N_d = \left(\frac{2}{e_0 \varepsilon \varepsilon_0 A^2}\right)\left[\frac{d\left(\frac{1}{C^2}\right)}{dV}\right]^{-1}$$

$$E - E_{FB} - \left(\frac{kT}{e}\right) = 0, \ E_{FB} = E - \left(\frac{kT}{e}\right)$$

Herein, $\varepsilon_0 = 8.854 \times 10^{-14} F \cdot cm^{-1}$

$e = 1.6 \times 10^{-19} C$, assume $T = 300$ K

$$\frac{kT}{e} = 8.617 \times 10^{-5} \times 300 = 0.026 \text{ eV}$$

$$A = 0.196 \text{ cm}^2$$

For N_2-annealed $CuInS_2$ curve in Figure 5c,

$$\text{slope} = \frac{d\left(\frac{1}{C^2}\right)}{dV} = \frac{2}{e_0 \varepsilon \varepsilon_0 N_d A^2} = \frac{3.755 - 2.45}{0 - (-0.2)} \times 10^7 \ F^{-2} V^{-1} = 6.53 \times 10^7 \ F^{-2} V^{-1}$$

When Y = 0, the intersection with X-axes is: E = -0.6 V vs. Ag/AgCl

The flat-band potential is:

$$E_{FB} = E - \left(\frac{kT}{e}\right) = -0.6 - 0.026 = -0.626 \text{ V vs. Ag/AgCl}$$

For H_2-annealed $CuInS_2$ curve in Figure 5d,

$$\text{slope} = \frac{d\left(\frac{1}{C^2}\right)}{dV} = \frac{2}{e_0 \varepsilon \varepsilon_0 N_d A^2} = \frac{1.45 - 0.71}{0 - (-0.7)} \times 10^7 \ F^{-2} V^{-1} = 1.06 \times 10^7 \ F^{-2} V^{-1}$$

When Y=0, the intersection with X-axes is: E = -1.18 V vs. Ag/AgCl

The flat-band potential is:

$$E_{FB} = E - \left(\frac{kT}{e}\right) = -1.18 - 0.026 = -1.206 \text{ V vs. Ag/AgCl}$$