Optimization of the processing parameters for the preparation of dip-coated CuO photocathodes and modification with Au nanoparticles for water-splitting

Nteseng D. M. Mosalakgotla¹, Pannan I. Kyesmen¹ and Mmantsae Diale¹ ¹Department of Physics, University of Pretoria, Private Bag X20, Hatfield 0028, South Africa Corresponding author e-mail addresses: pannan.kyesmen@up.ac.za: mmantsae.diale@up.ac.za



Fig. S1. FE-SEM micrographs of CuO thin films consisting of (a) 5, (b) 7, and (c) 10 layers with the insets showing the histograms of their particle size distribution, respectively: (d) shows the surface morphology of CuO/Au films.



Fig. S2. FE-SEM micrographs of CuO thin films annealed at different temperatures of (a) 400° C, (b) 500° C (c) 600° C and (d) 650° C together with the corresponding histograms of their particle size distribution.



Fig. S3. FE-SEM Cross-sectional views of CuO thin films consisting of (a) 5 layers, (b) 7 layers (c) 10 layers, and (d) 7 layers/Au respectively.

Table S1. Summary of the film thickness estimated for CuO/Au films and the CuO samples prepared at various withdrawal velocities and number of film layers.

Sample	Thickness (nm)	
50 mm	239.7 ± 23	
100 mm	277.3 ± 32	
150 mm	317.4 ± 40	
200 mm	355.2 ± 22	
CuO-5L	317.4 ± 40	
CuO-7L	432.8 ± 27	
CuO-10L	693.6 ± 35	
CuO-7L-Au	55.8 ± 12	



Fig. S4. EDS analysis of CuO thin films consisting of (a) 5 Layers, (b) 7 Layers, (c) 10 layers and (d) 7 Layers/Au respectively.



Fig. S5. EDS analysis of CuO thin films annealed at different temperatures of (a) 400 °C (b) 500 °C (c) 600 °C and (d) 650 °C.

Table S2. The approximate flat-band potential and charge carrier concentration values calculated for the CuO and CuO/Au photocathodes.

Sample	V _{fb} vs RHE (V)	N _D * 10 ²⁰ (cm ⁻³)
7 Layers	1.049	0.90
7 Layers/Au	0.877	5.64

The flat-band potential and charge carrier concentration were calculated for the CuO and CuO/Au photocathodes using the Mott-Schottky relation in Eq. S1:

$$\frac{1}{c^2} = \frac{-2}{\varepsilon \varepsilon_0 e A^2 N_A} \left(V - V_{FB} + \frac{kT}{e} \right)$$
 Eq. S1

where C is the capacitance of the space-charge layer, ε is the dielectric constant of the material, ε_0 is the vacuum permittivity with a numerical value of 8.85 x 10⁻¹⁴ F/cm and *e* is the electronic charge with a value of 1.602 x 10⁻¹⁹ C, A is the surface area of the electrode, N_A is the acceptor density, V represent the applied voltage, V_{FB} is the flat-band potential, K is the Boltzmann constant, and T stands for the temperature.