

Supporting Information

Untapped Potential of Scrap Brass Alloy: A New Frontier in the Use of Brass-Based Photocathodes for Stable and Durable Photoelectrochemical Water Splitting

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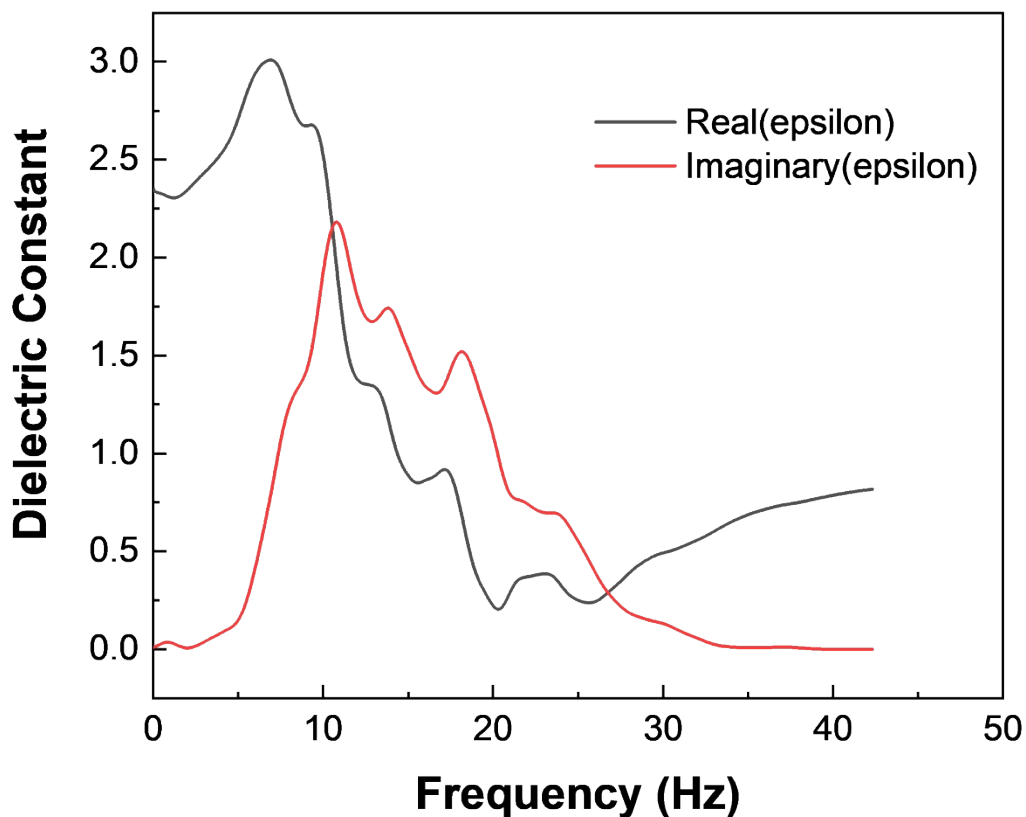


Figure S1. Dielectric Function of CuZnO.

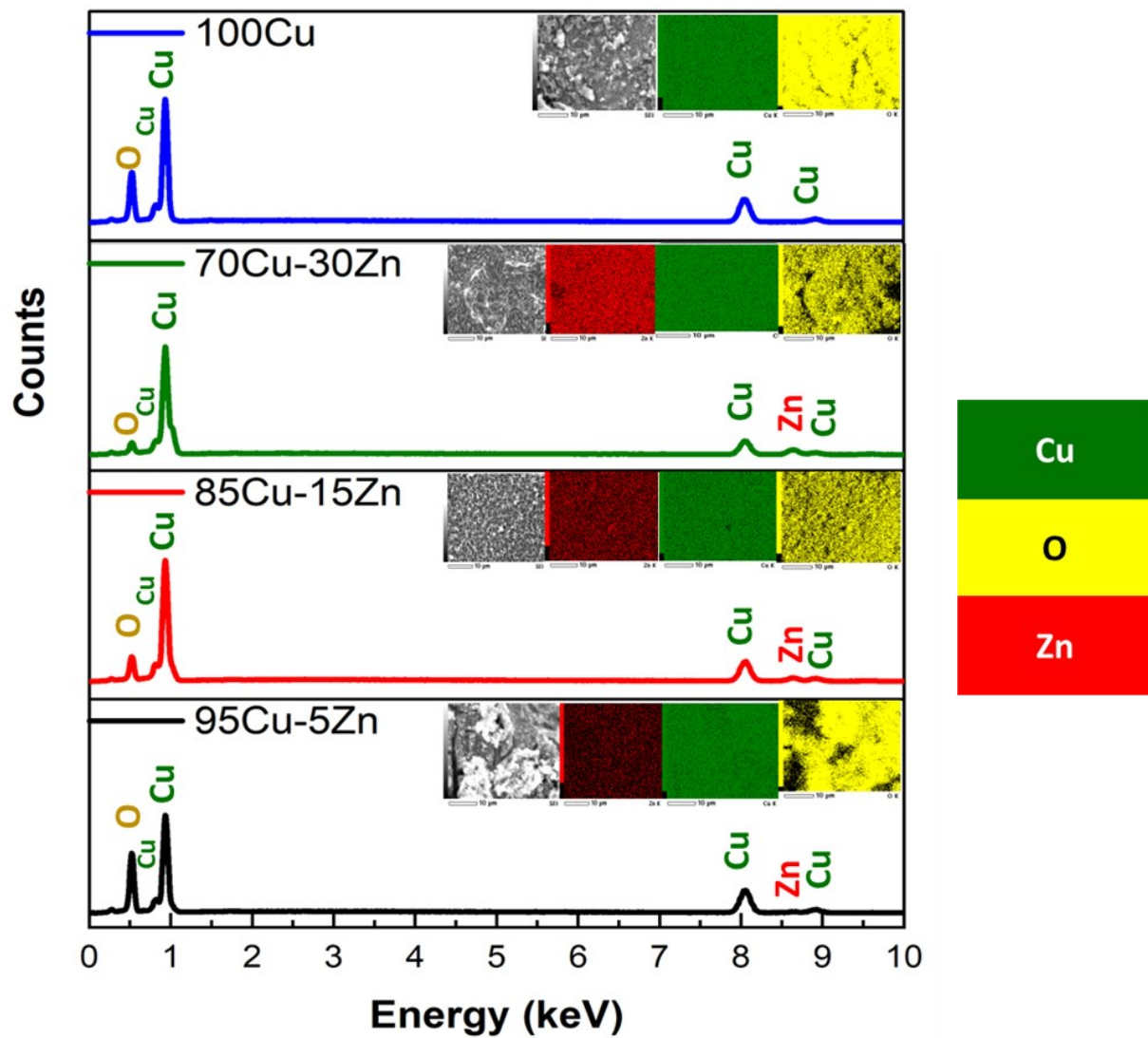


Figure S2. Elemental mapping of the samples after being anodized.

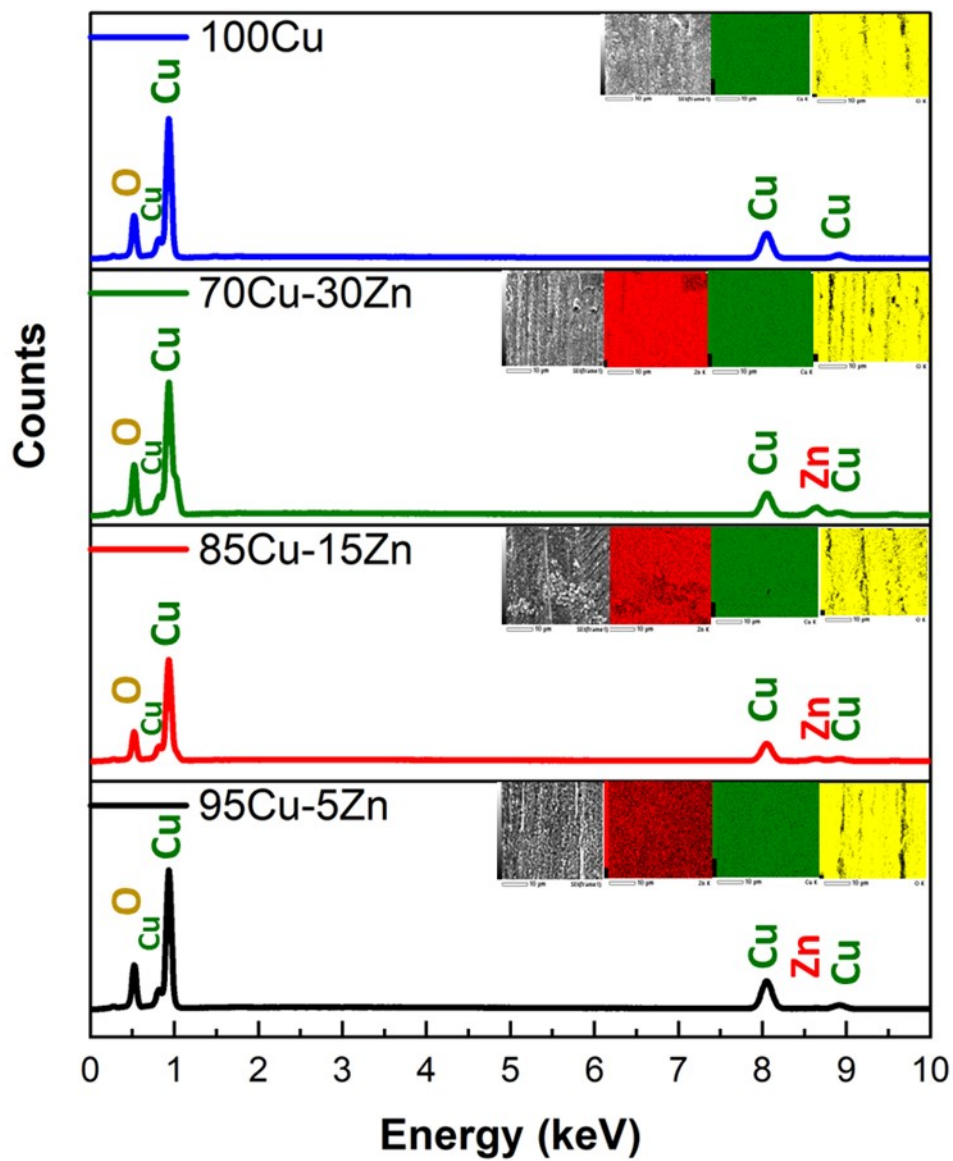


Figure S3. Elemental mapping of the samples after being annealed.

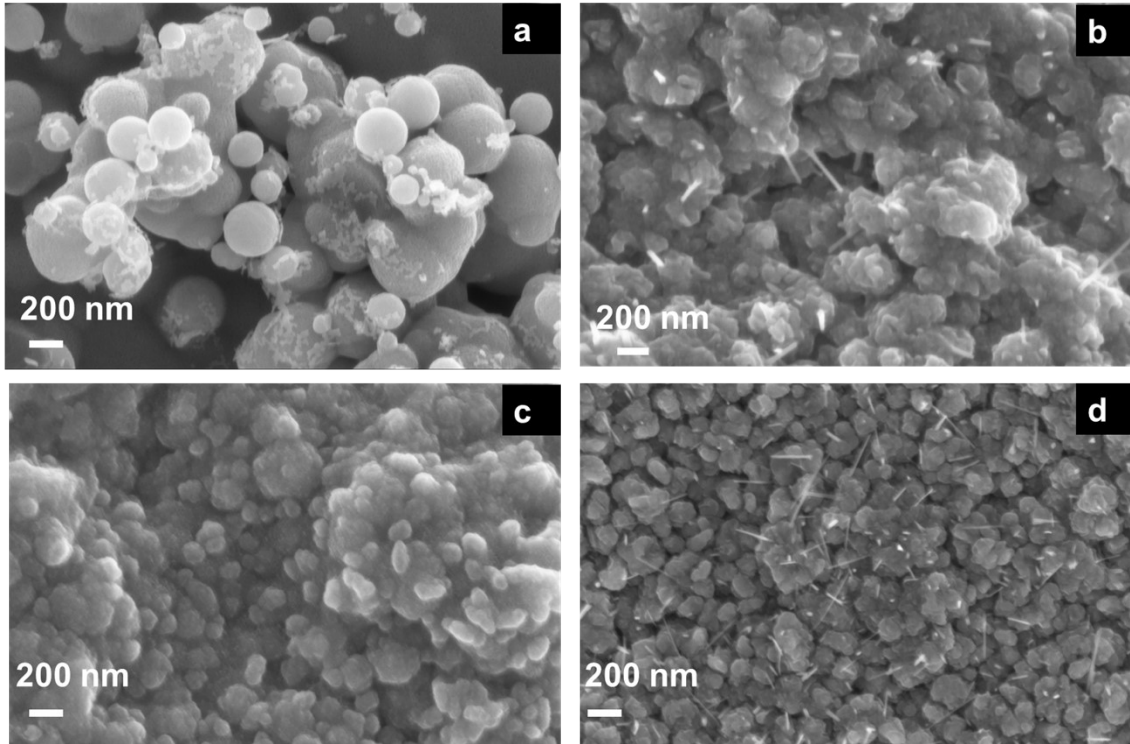


Figure S4. (a) Top-view SEM images of the as-anodized (a) 95Cu-5Zn, (b) 85Cu-15Zn, (c) 70Cu-30Zn, and (d) 100Cu samples.

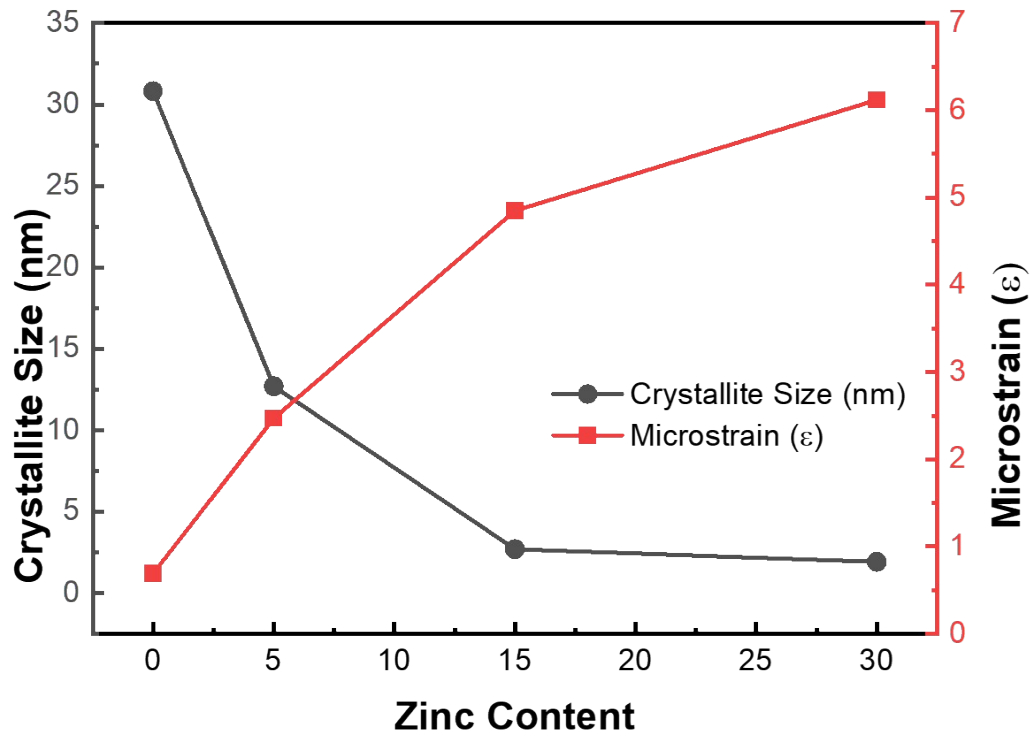


Figure S5. Crystallite size and microstrain vs Zinc content.

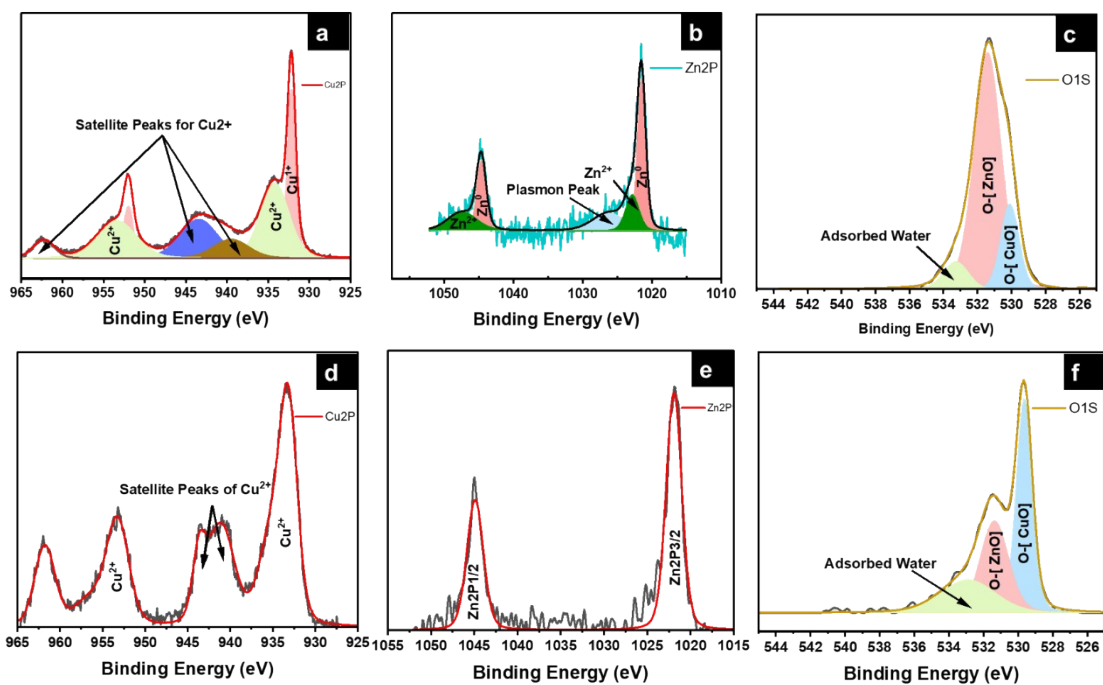


Figure S6. High-Resolution XPS results for as-anodized (a,b,c), and as-annealed (d,e,f) 85Cu-15Zn sample.

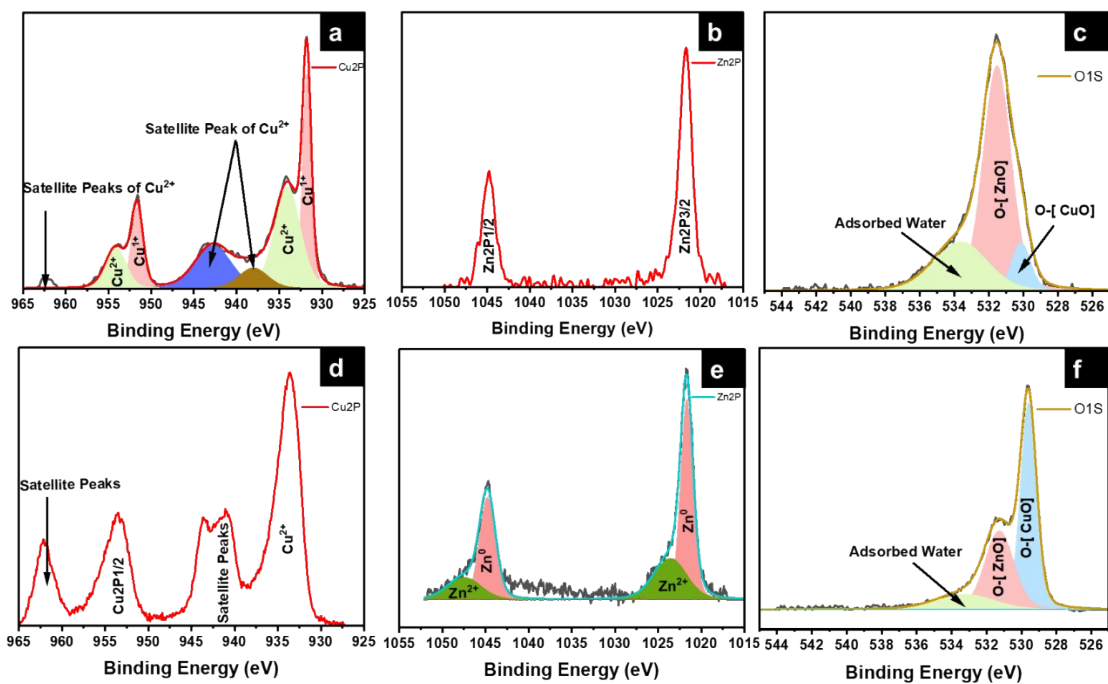


Figure S7. High Resolution XPS results for as-anodized (a,b,c), and as-annealed (d,e,f) 70Cu-30Zn sample.

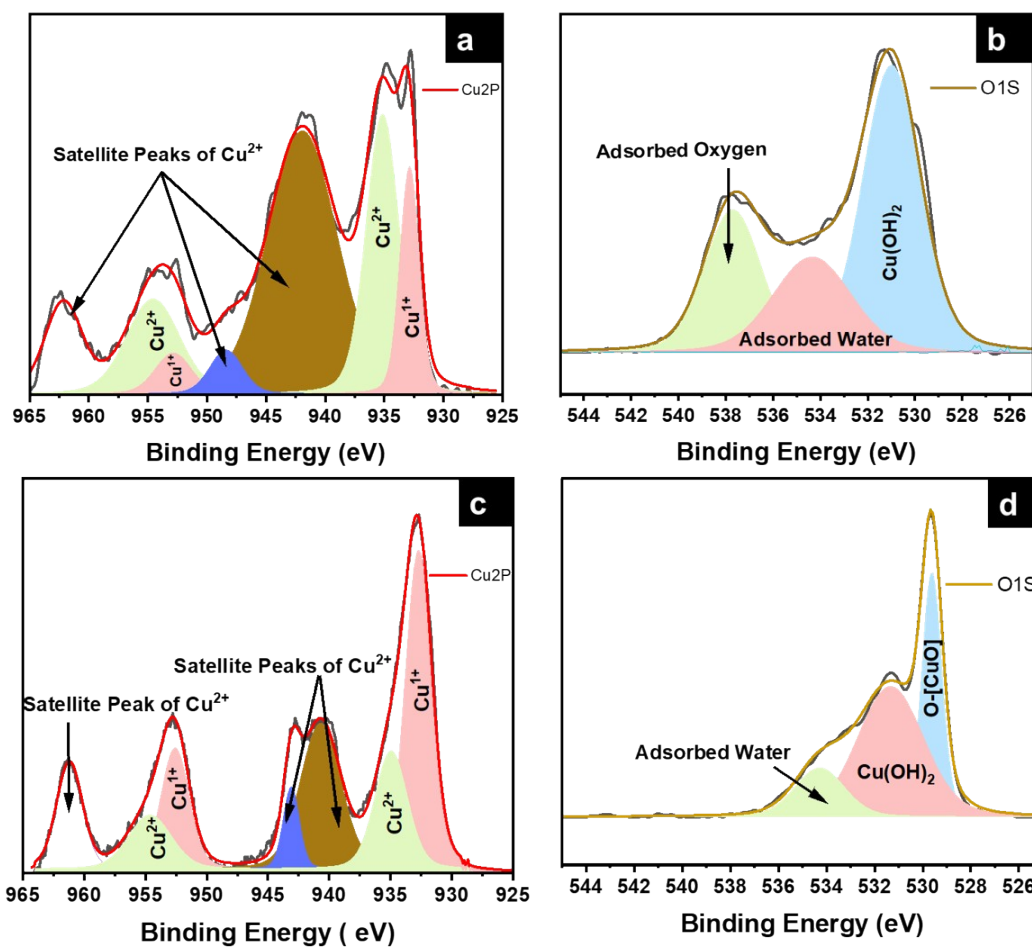


Figure S8. High-Resolution XPS results for as-anodized (a,b), and as-annealed (c,d) 100Cu sample.

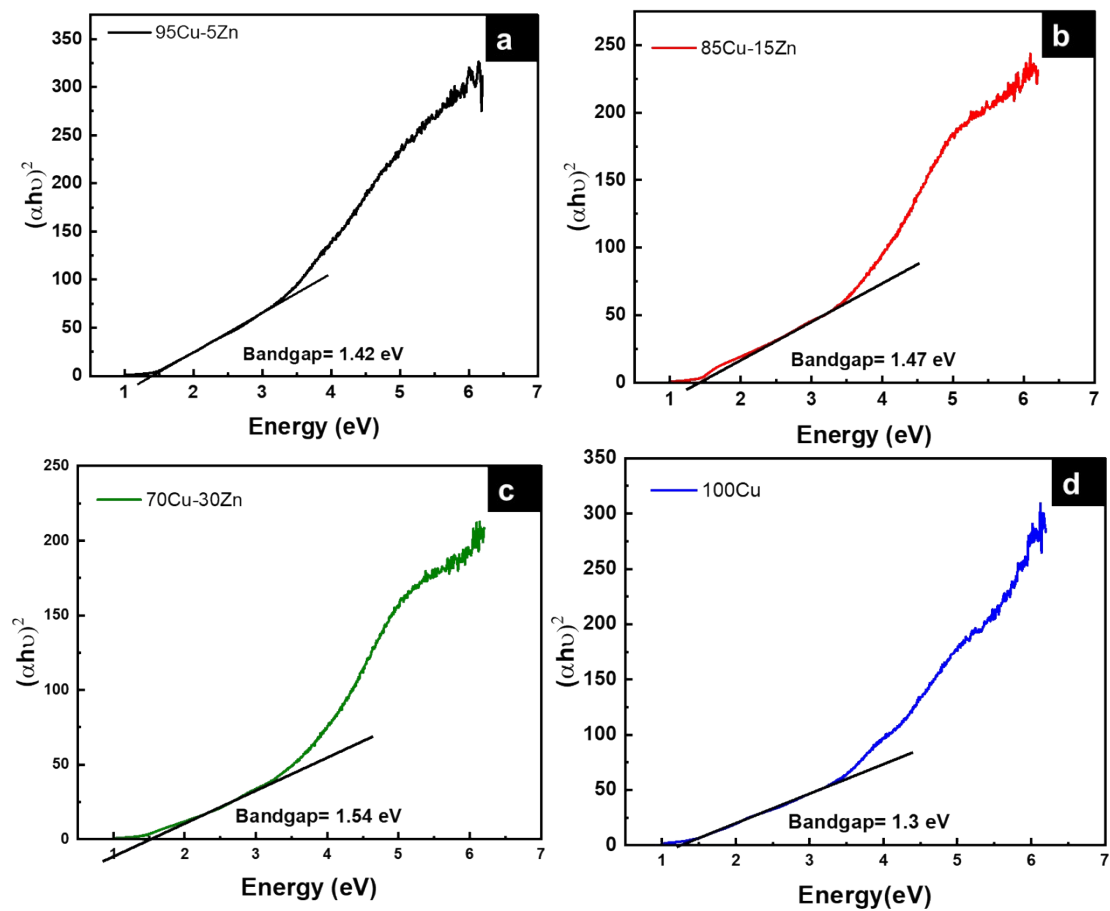


Figure S9. Band gap calculations for the (a) 95Cu-5Zn sample, (b) 85Cu-15Zn sample, (c) 70Cu-30Zn sample, and (d) 100 Cu samples.

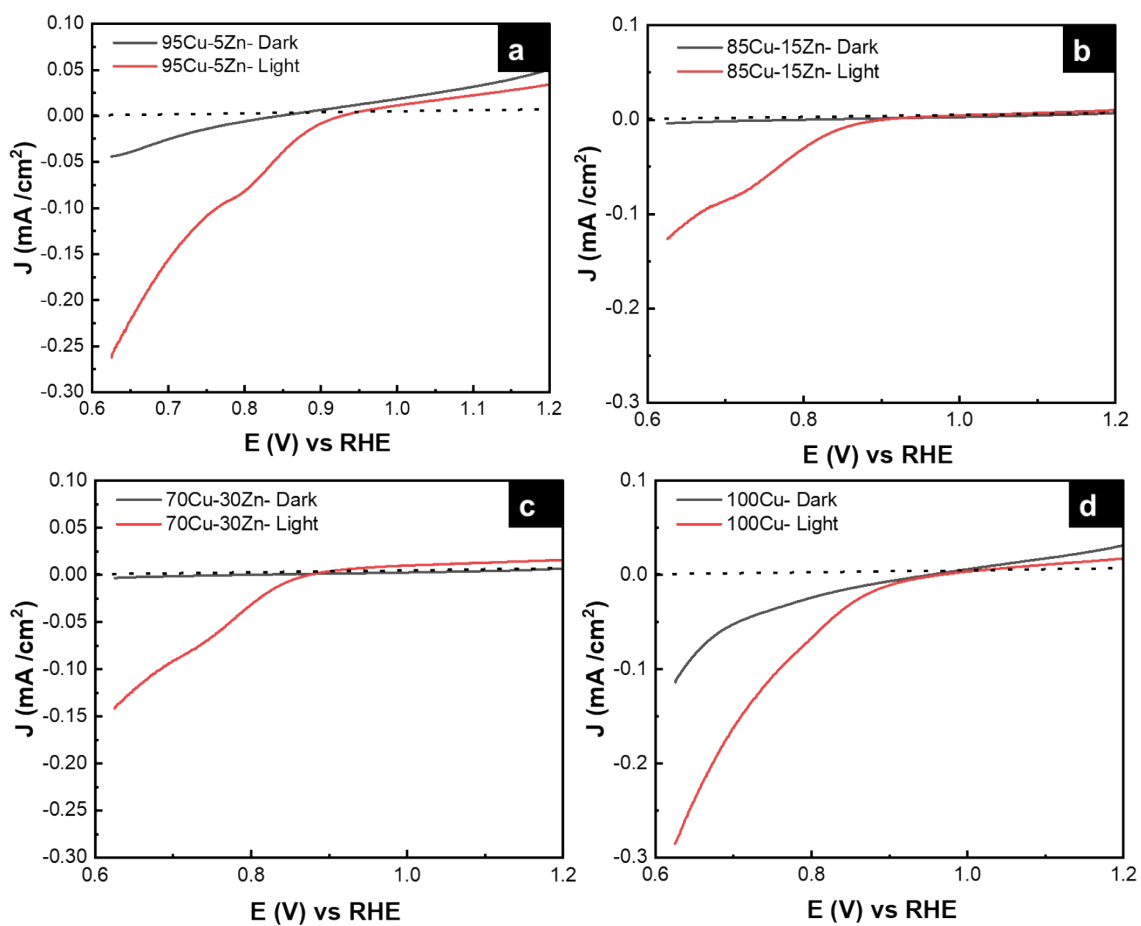


Figure S10. Linear sweep voltammetry (LSV) graphs for (a) 95Cu-5Zn, (b) 85Cu-15Zn, (c) 70Cu-30Zn, (d) 100Cu.

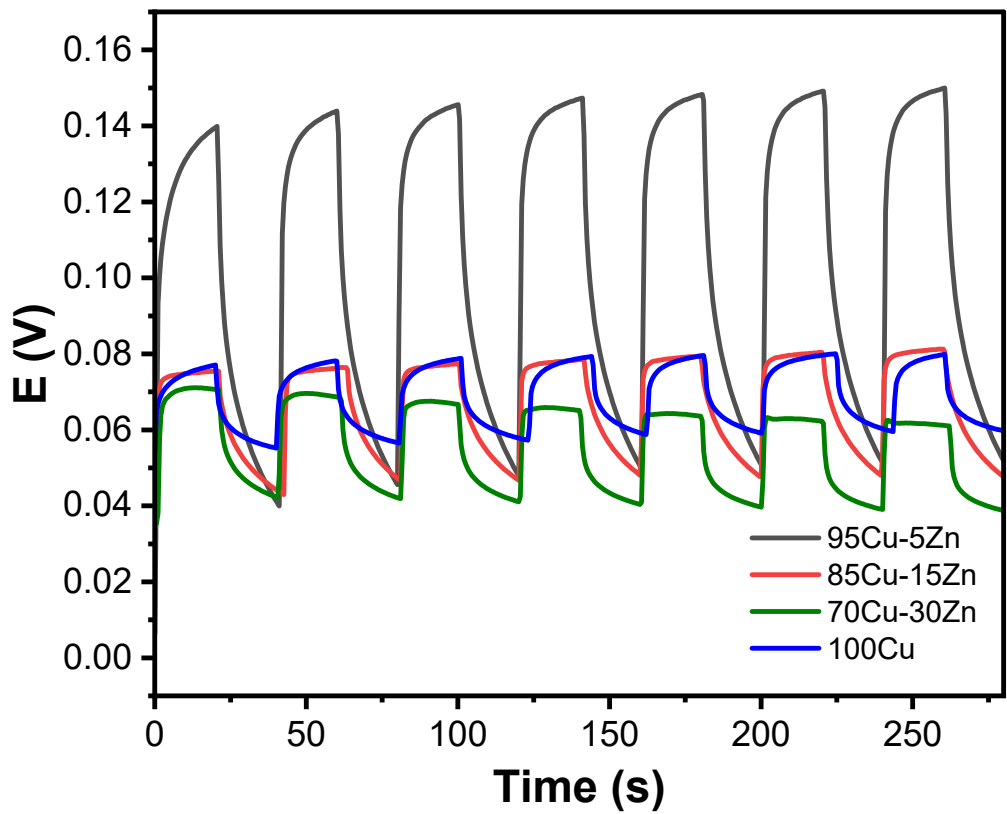


Figure S11. Open circuit potential (OCP) measurements while chopping illumination.

Electrochemical Impedance Spectroscopy:

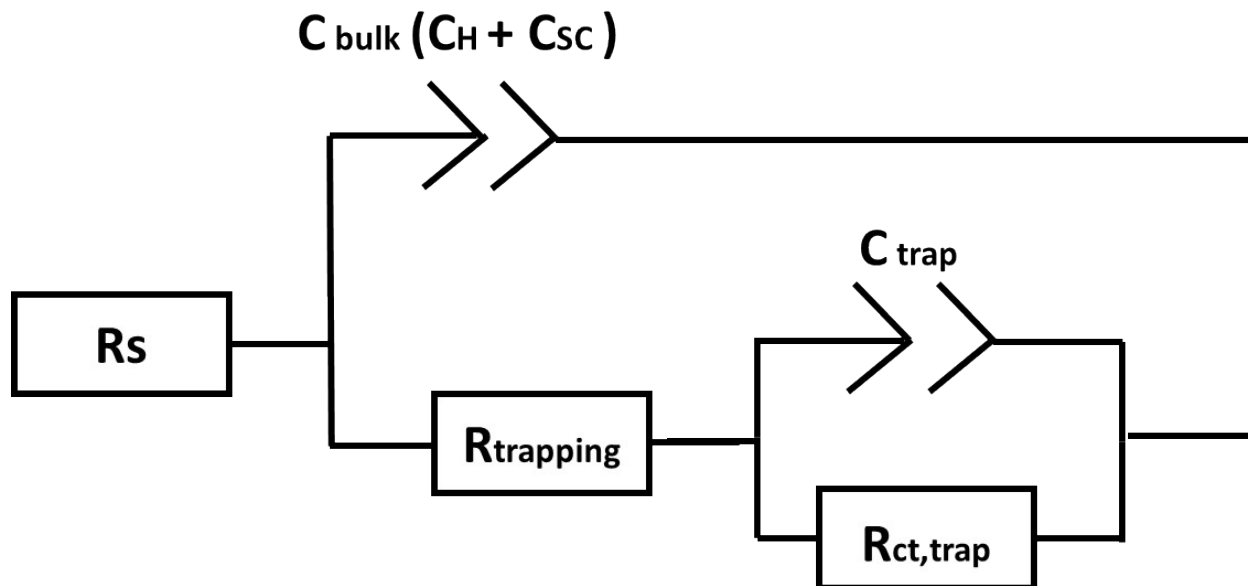


Figure S12. Equivalent circuit for electrochemical impedance spectroscopy data fitting.

Figure S12 shows the equivalent circuit used to fit the EIS data, where R_s is the solution resistance and the resistance related to the wires and connections, C_{bulk} is the capacitance of the bulk, C_{sc} is the capacitance of the space charge layer inside the semiconductor, and C_H is the capacitance of the Helmholtz layer inside the electrolyte ($C_{\text{bulk}}^{-1} = C_{sc}^{-1} + C_H^{-1}$), R_{trapping} is related to the charge trapping and detrapping at the surface states, $R_{\text{ct, trap}}$ is associated with the charge transfer resistance from the surface states to the electrolyte, and C_{trap} related to the capacitive effect induced by charge accumulation in surface states. This equivalent circuit was used to fit the data in dark and under illumination, as shown in **Figure S13**.

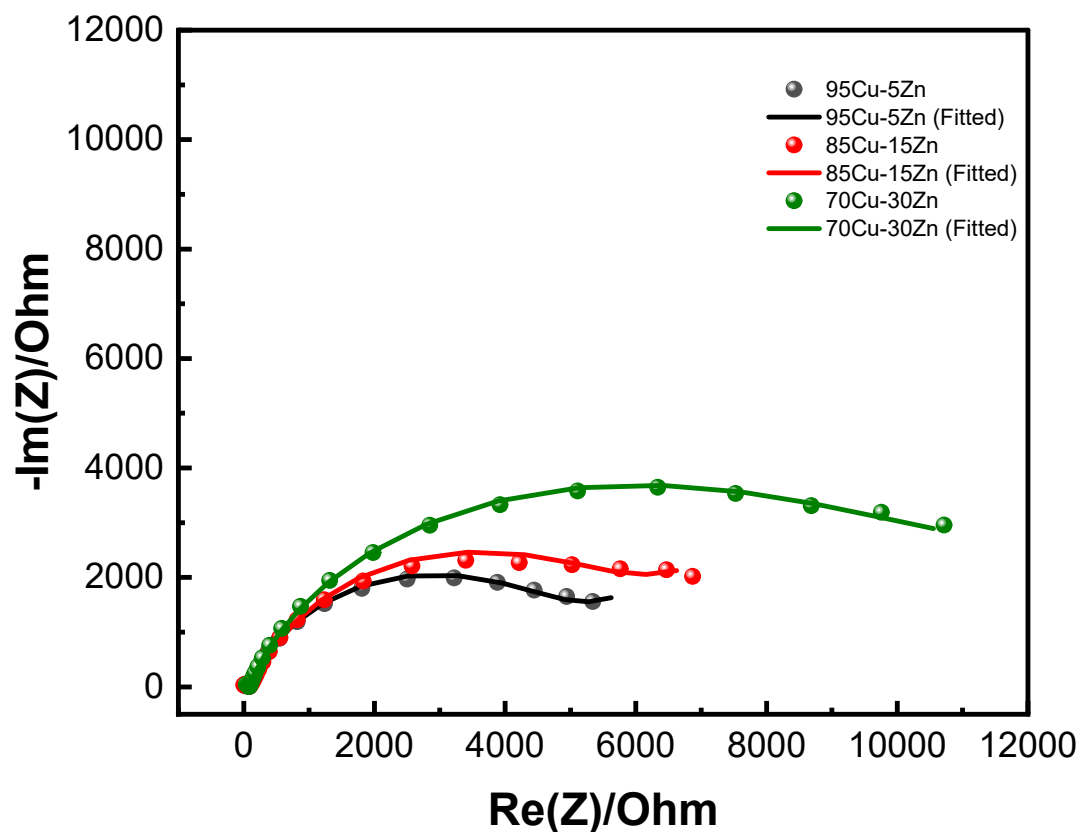


Figure S13. EIS Data under illumination at 0.62 V vs RHE.

To get more insight into the trapping of charges on the surface and to prove the existence of surface states, C_{trap} values at low frequencies are shown in **Figure S12 and Figure S 13**. The low frequency guarantees the low contribution of C_{bulk} . Therefore, we have chosen the frequency of 50 mHz to get the value of C_{trap} versus applied potential. In the dark and under illumination,

C_{trap} shows a Gaussian peak for all samples shown through the fitting of the sample to a Gaussian function, which is a proof of the existence of surface states at around 0.8 V vs RHE.

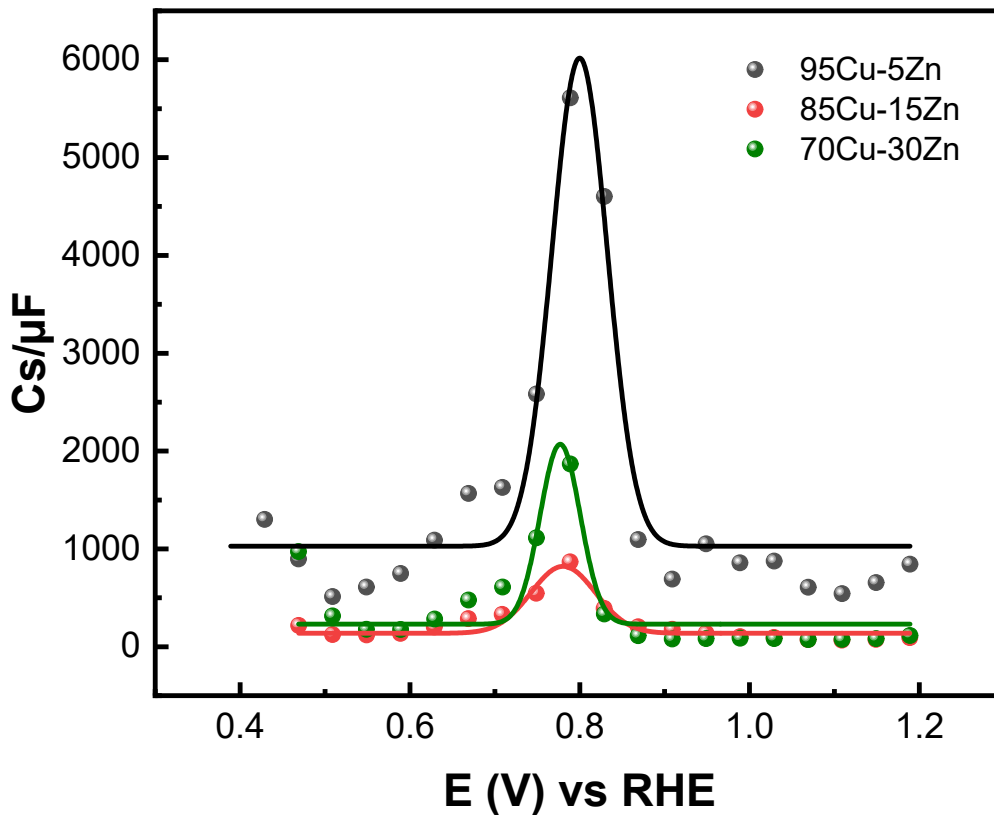


Figure S14. Capacitance versus applied potential graph in the dark.

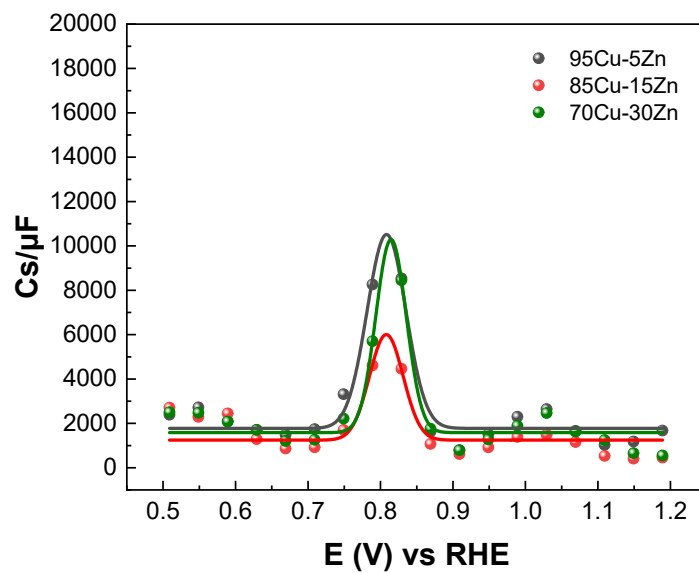


Figure S15. Capacitance versus applied potential graph under illumination.

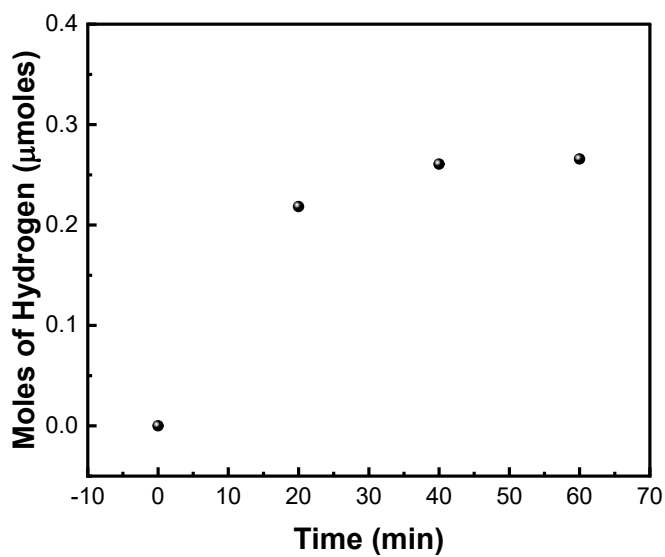


Figure S16. Amount of hydrogen produced within 60 minutes of continuous illumination by 95Cu-5Zn sample.

Table S1. The amount of hydrogen obtained upon the use of Cu-based photocathodes under close conditions to the ones used in our study.

Photocathode	Experimental Conditions	Amount of Hydrogen evolved
CuFe _x O _y <i>Green Chemistry</i> , 2020, 22 , 3141–3149	Applying constant current of 10μA	4.8 nmol cm ⁻² (after one hour of continuous illumination)
Carbon coated Cu ₂ O nanowires <i>Appl Surf Sci</i> , 2015, 358 , 404–411	At 0 V vs RHE	~ 6 μmol cm ⁻² (after 16.6 min of continuous illumination)
Li incorporated in CuAl ₂ O ₄ <i>J Catal</i> , 2021, 400 , 218–227	Applying a constant voltage of 0.4V vs RHE	~ 0.27 μmol cm ⁻² (after one hour of continuous illumination)
Li doped CuO <i>Nanoscale</i> , 2020, 12 , 7766–7775	Applying a constant voltage of 0.3 V vs RHE	~ 0.2 nmol L ⁻¹ (after 15 minutes of continuous illumination)
Cu-Zn This work	Applying a constant voltage of 0.6 V vs RHE	1.06 μmol cm⁻² (after one hour of continuous illumination)