

SUPPLEMENTARY INFORMATION

Figure S1 - XRD analysis

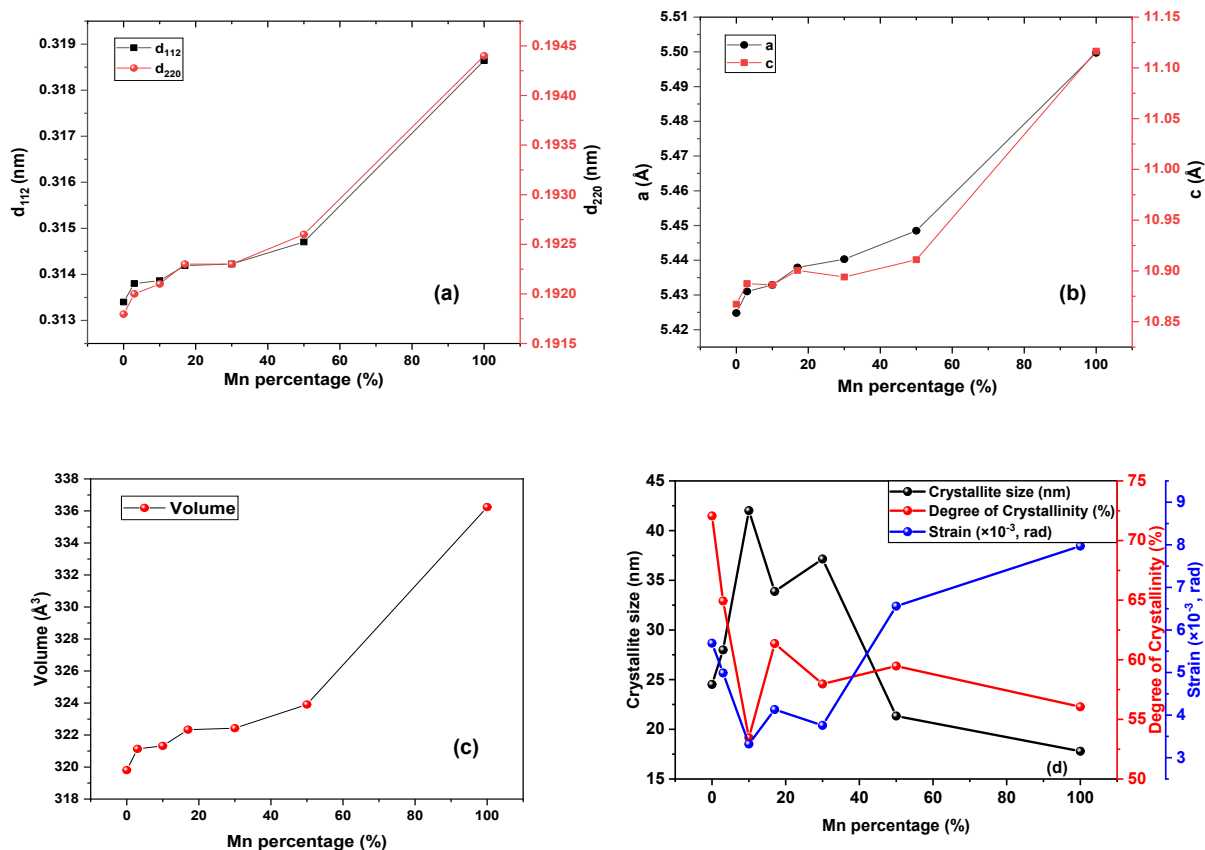


Figure S1 (a) interplanar spacing for various Mn percentages, (b) Lattice parameters ‘a’ and ‘c’ for Mn doped CZTS samples, and (c) volume for Mn doped CZTS samples (d) crystallite size, degree of crystallinity, and strain for Mn doped CZTS samples.

Table S1. The crystallite size and strain for Williamson-hall method, Scherrer method and modified Scherrer method and calculated strain values to identify nature of strain

| Sample (Zn:Mn) percentage ratio | Williamson–Hall method | | Scherrer Method | | Modified Scherrer method | Nature of strain calculation | | |
|--|---------------------------------------|--|---------------------------------------|--|---------------------------------------|------------------------------|--------------|-----------------------------|
| | Crystallite Size (<i>D</i>) (nm) | Strain, $\epsilon \times 10^{-3}$ (rad) | Crystallite Size (<i>D</i>) (nm) | Strain, $\epsilon \times 10^{-3}$ (rad) | Crystallite Size (<i>D</i>) (nm) | $K(d_{112})$ | $K(d_{220})$ | Avg. strain (<i>K</i>) |
| S0 (100:0) | 31.45 | 1.75 | 24.52 | 5.69 | 21.10 | 0 | 0 | 0.0000 |
| S1 (97:3) | 36.56 | 1.17 | 27.99 | 4.99 | 29.72 | 0.0013 | 0.0010 | 0.0012 |
| S2 (90:10) | 103.87 | 1.97 | 42.01 | 3.32 | 48.08 | 0.0015 | 0.0016 | 0.0015 |
| S3 (83:17) | 40.21 | 1.02 | 33.88 | 4.13 | 31.62 | 0.0025 | 0.0026 | 0.0026 |
| S4 (70:30) | 57.37 | 1.33 | 37.14 | 3.76 | 40.45 | 0.0026 | 0.0026 | 0.0026 |
| S5 (50:50) | 24.48 | 0.93 | 21.34 | 6.56 | 21.78 | 0.0042 | 0.0042 | 0.0042 |
| S6 (0:100) | 20.59 | 2.43 | 17.79 | 7.97 | 15.58 | 0.0167 | 0.0136 | 0.0151 |

Figure S2 - BET analysis

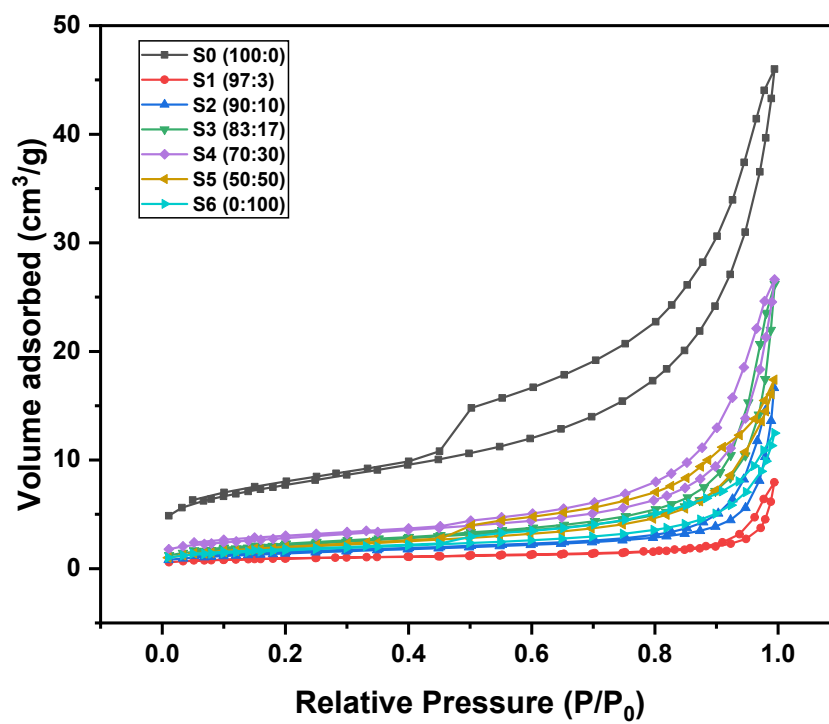


Figure S2. BET-N₂ adsorption-desorption isotherm

Table S2: Surface area and pore size for all anode samples.

| Sample (Zn:Mn) percentage ratio | BET Surface area, m²/g | Langmuir Surface area, m²/g | Adsorption pore size, nm | Desorption pore size, nm | adsorption pore volume (cm³/g) | desorption pore volume (cm³/g) |
|--|--|---|-------------------------------------|-------------------------------------|--|--|
| S0 (100:0) | 27.5130 | 53.3894 | 7.1012 | 8.6385 | 0.0488 | 0.0594 |
| S1 (97:3) | 3.3603 | 6.3028 | 5.1224 | 6.9673 | 0.0043 | 0.0059 |
| S2 (90:10) | 5.0669 | 11.1901 | 7.0569 | 10.9467 | 0.0089 | 0.0139 |
| S3 (83:17) | 7.8286 | 16.3453 | 8.4935 | 11.6504 | 0.0166 | 0.0228 |
| S4 (70:30) | 10.0245 | 21.1536 | 8.7884 | 11.9997 | 0.0220 | 0.0301 |
| S5 (50:50) | 7.0641 | 15.9444 | 9.6853 | 11.3034 | 0.0171 | 0.01996 |
| S6 (0:100) | 6.0252 | 12.5485 | 7.3430 | 8.8983 | 0.0111 | 0.0134 |

Figure S3. DLS analysis

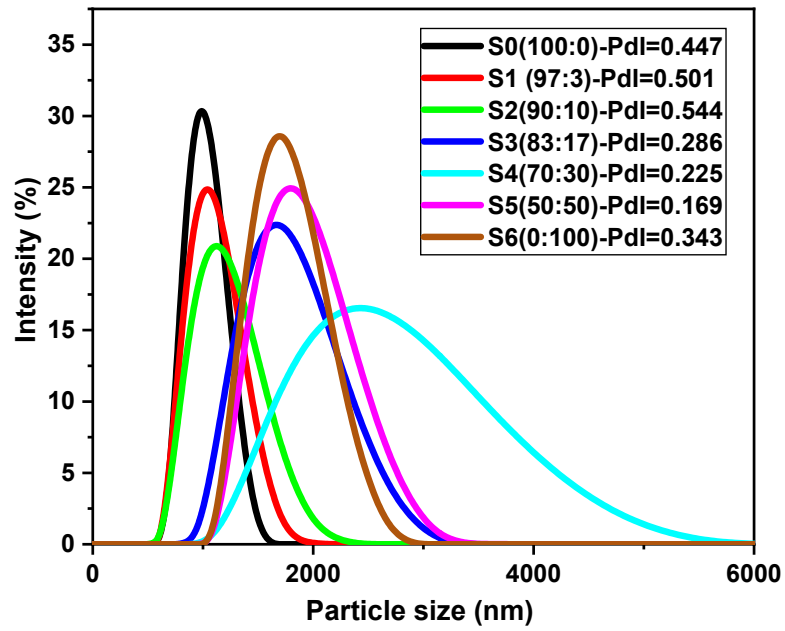


Figure S3. particle size distribution from DLS measurements