

# Unraveling the Effect of Compositional Ratios on the Kesterite Thin-Film Solar Cells Using Machine Learning Techniques

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**Table S1.** Categories of the different device parameters from the  $\text{Cu}_2\text{ZnSn}(\text{S,Se})_4$  (CZTSSe) TFSCs.

| Statistical parameters | PCE (%)    | FF (%)      | $J_{sc}$ (mA/cm <sup>2</sup> ) | $V_{oc}$ (mV) | $R_s$ ( $\Omega$ ) | $R_{sh}$ ( $\Omega$ ) |
|------------------------|------------|-------------|--------------------------------|---------------|--------------------|-----------------------|
| Low                    | 5.01-6.53  | 38.00-48.00 | 24.00-29.40                    | 374.00-441.00 | 2.00-11.11         | 11.00-294.12          |
| Medium                 | 6.53-7.34  | 48.00-52.00 | 29.40-30.90                    | 441.00-459.00 | 11.11-13.50        | 294.12-470.50         |
| High                   | 7.34-8.16  | 52.00-56.00 | 30.90-32.21                    | 459.00-479.00 | 13.50-16.00        | 470.50-714.29         |
| Very- High             | 8.16-10.24 | 56.00-65.00 | 32.21-37.10                    | 479.00-529.00 | 16.00-45.40        | 714.29-5000           |

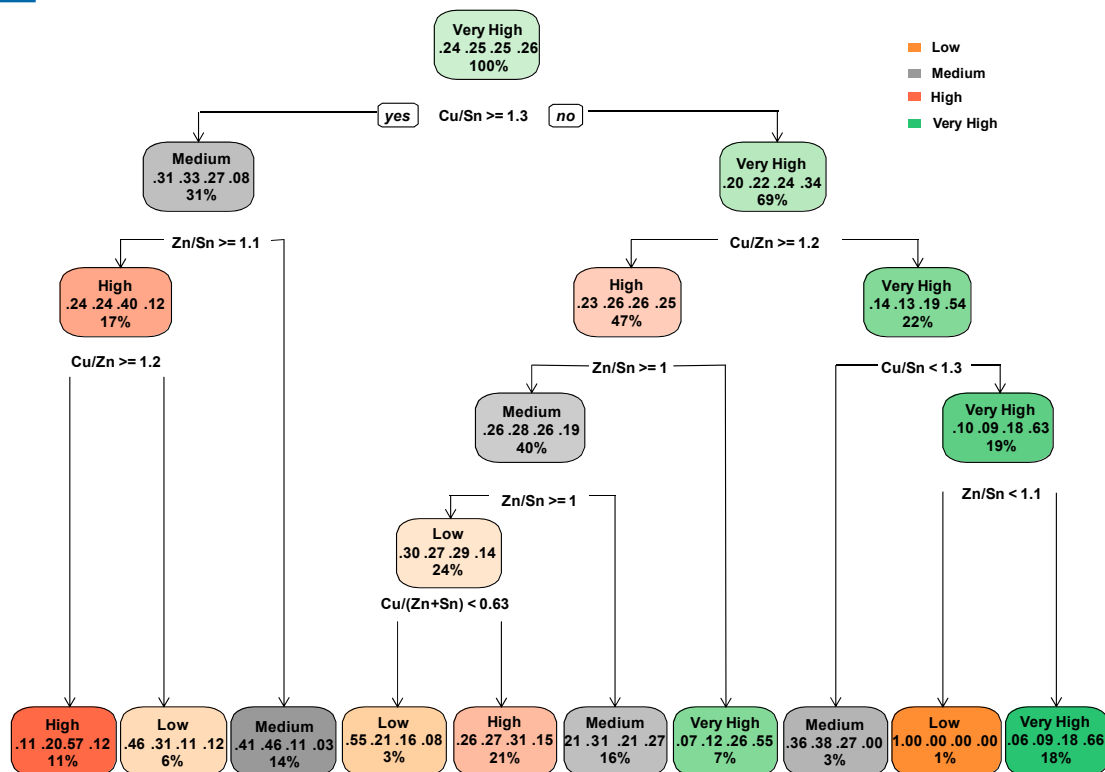


Figure S1: DT model for the FF of the CZTSSe TFSCs.

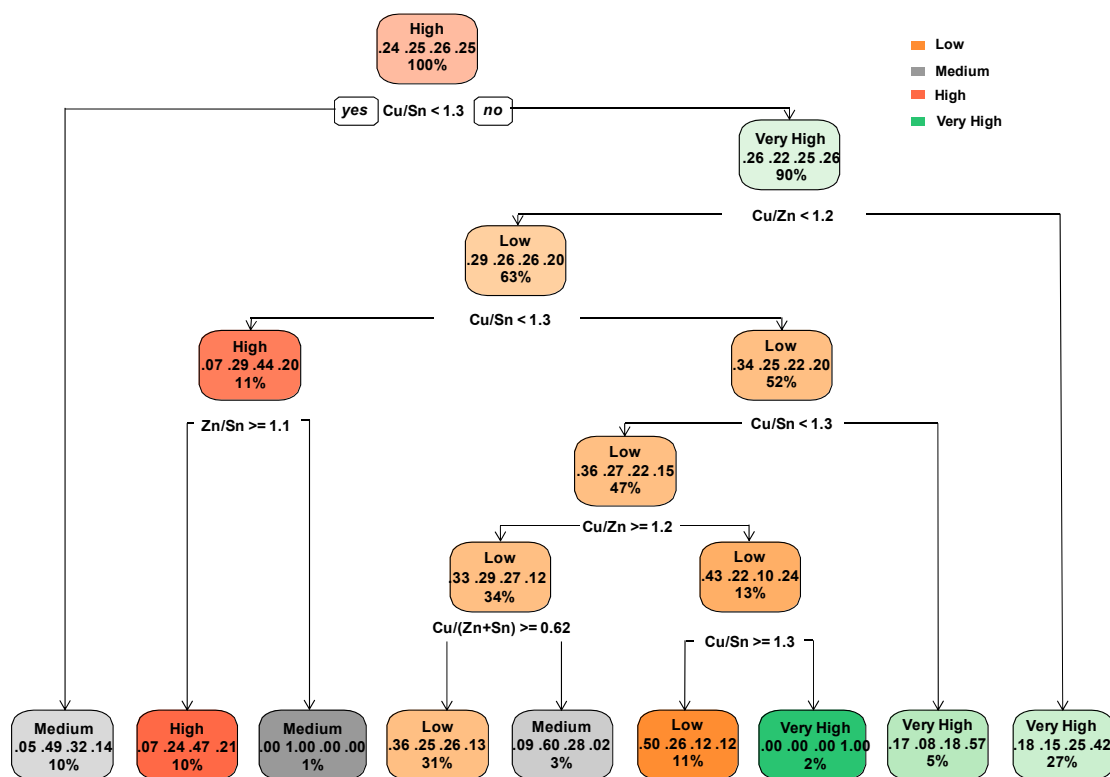


Figure S2: DT model for the  $J_{sc}$  of the CZTSSe TFSCs.

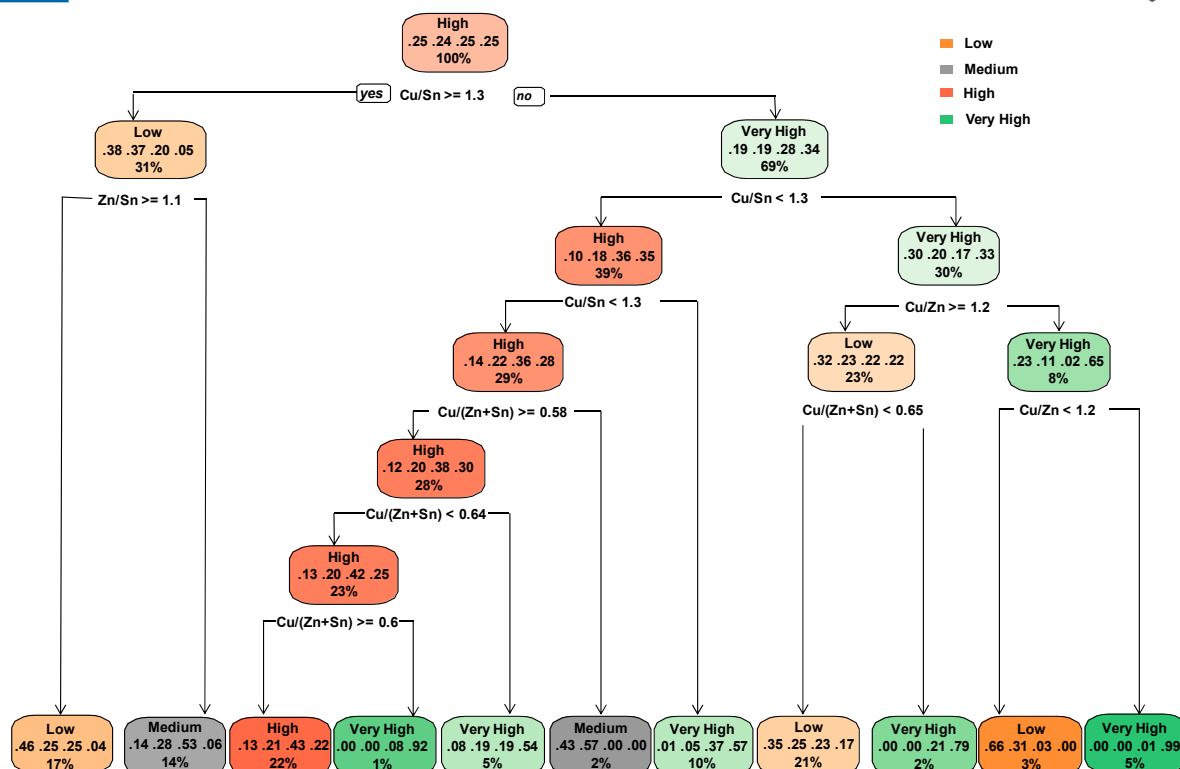


Figure S3: DT model for the  $V_{oc}$  of the CZTSSe TFSCs.

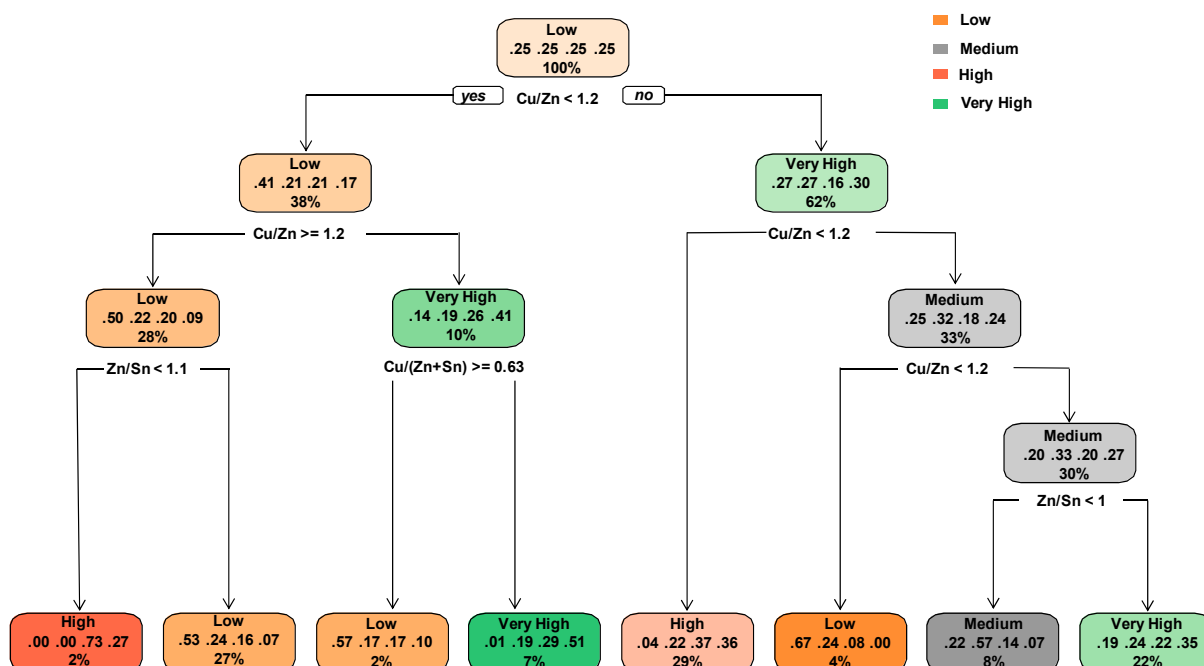


Figure S4: DT model for the  $R_s$  of the CZTSSe TFSCs.

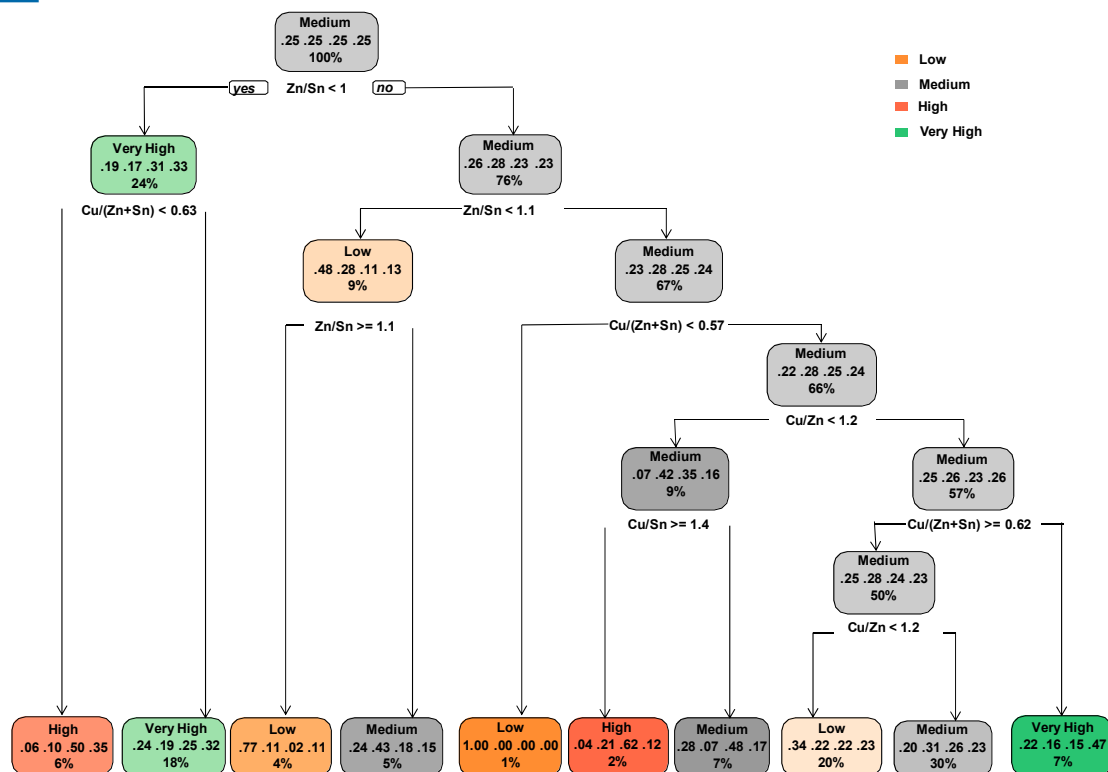


Figure S5: DT model for the  $R_{sh}$  of the CZTSSe TFSCs.

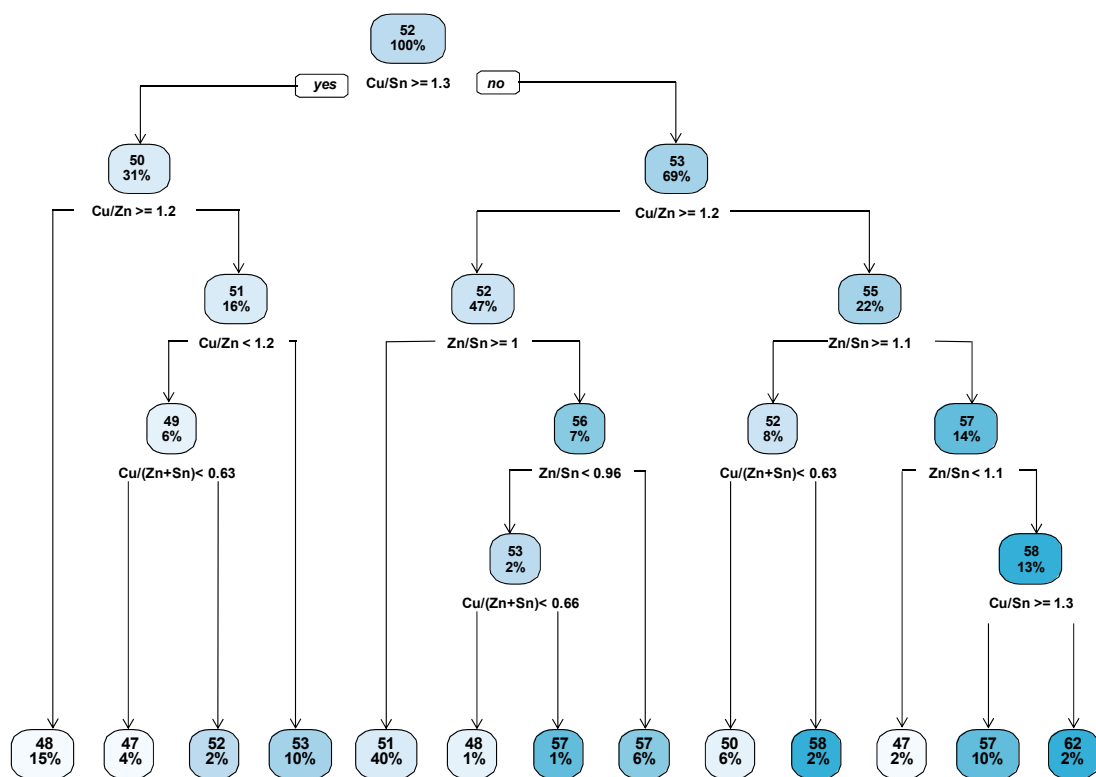
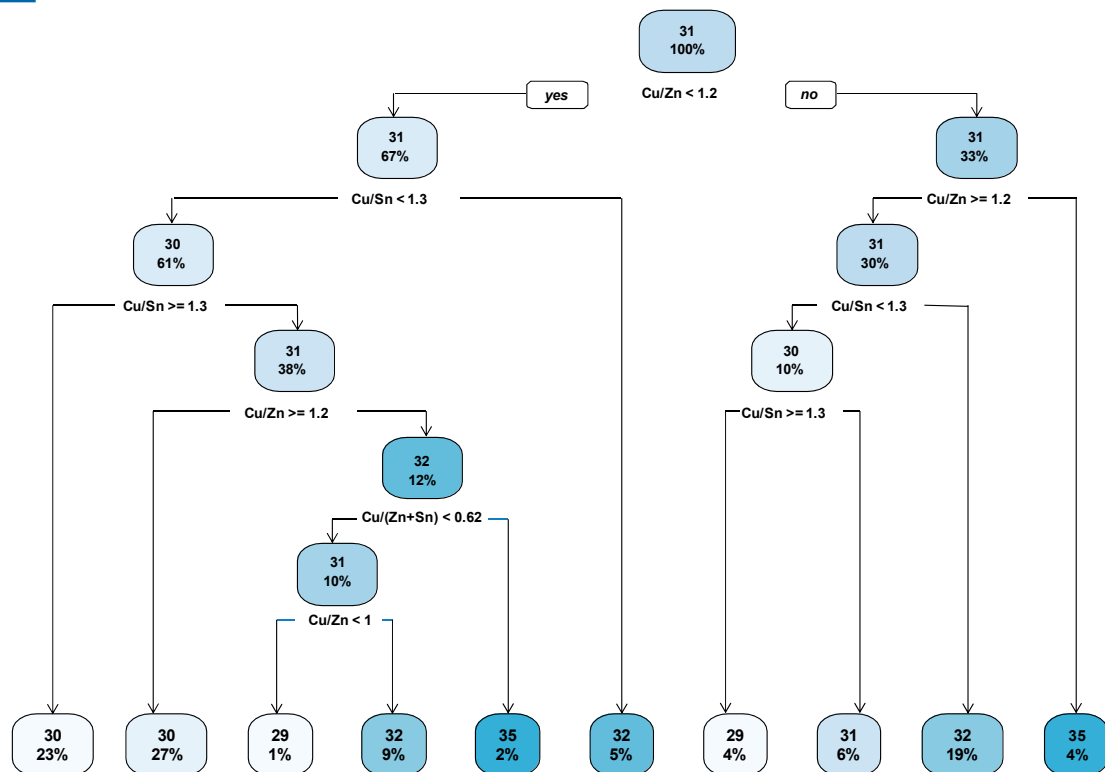
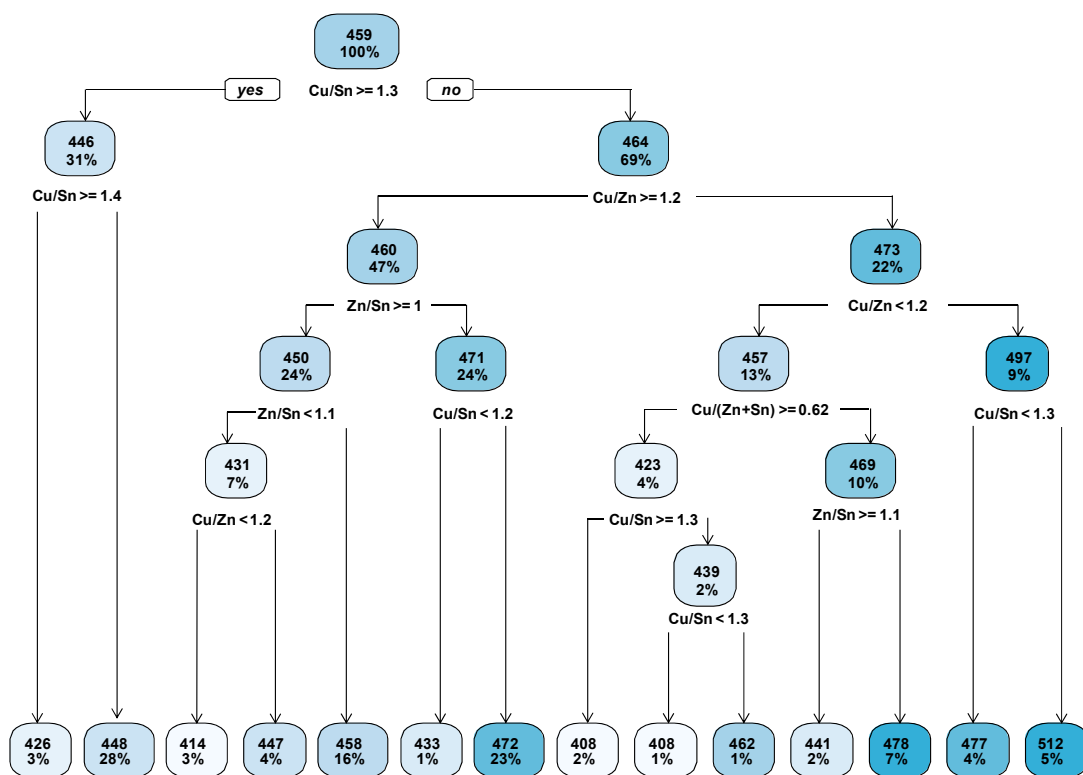


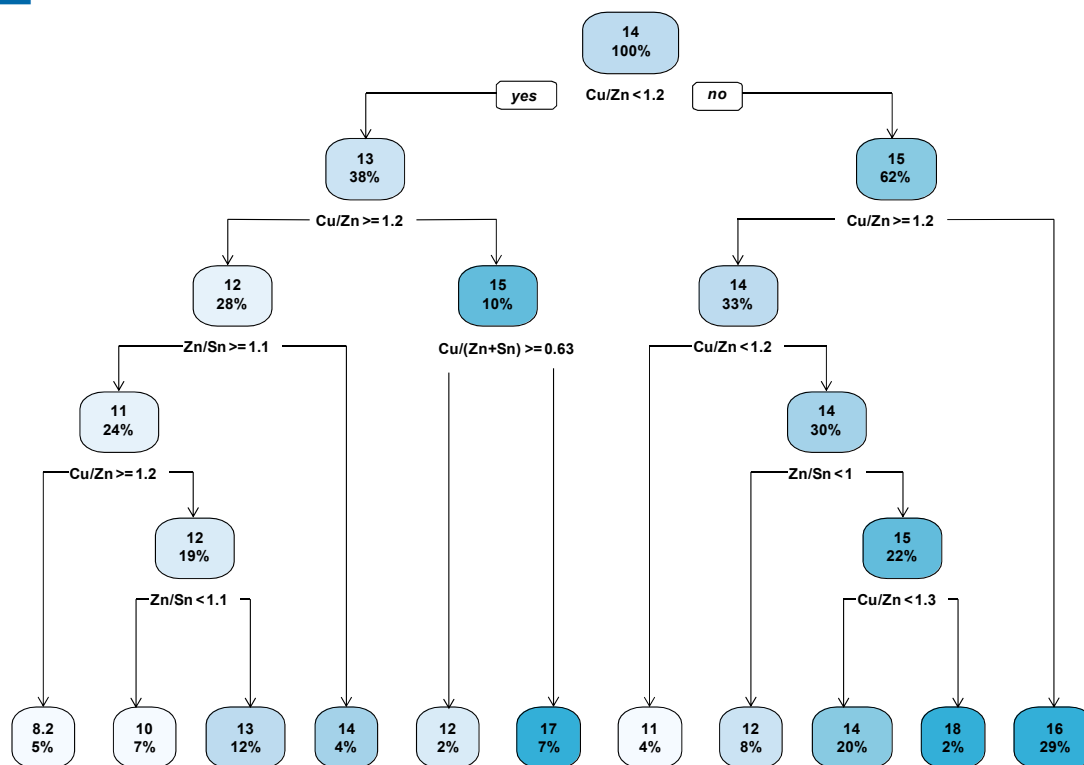
Figure S6: CART model for the FF of the CZTSSe TFSCs.



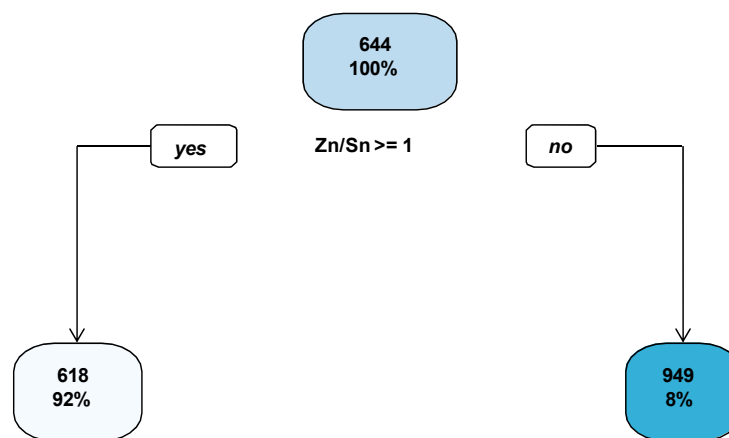
**Figure S7:** CART model for the  $J_{sc}$  of the CZTSSe TFSCs.



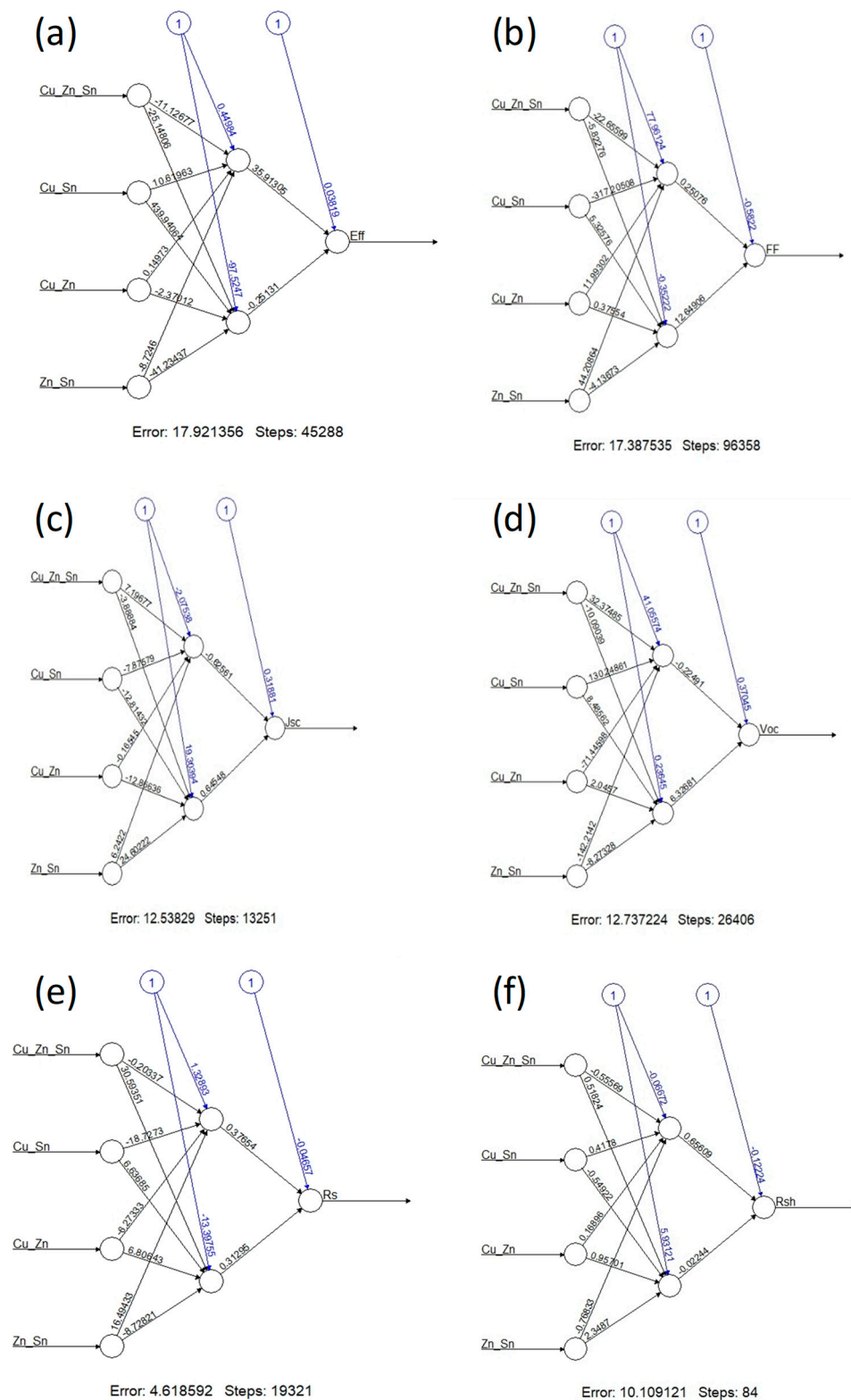
**Figure S8:** CART model for the  $V_{oc}$  of the CZTSSe TFSCs.



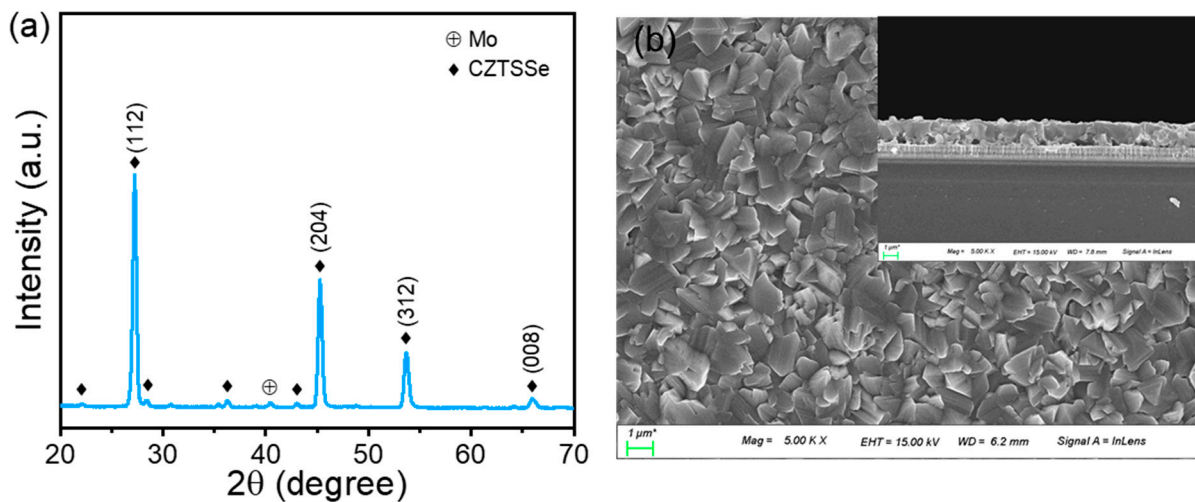
**Figure S9:** CART model for the  $R_s$  of the CZTSSe TFSCs.



**Figure S10:** CART model of the  $R_{sh}$  of the CZTSSe TFSCs.



**Figure S11:** ANN structure related to (a) PCE, (b) FF, (c) J<sub>sc</sub>, (d) V<sub>oc</sub>, (e) R<sub>s</sub>, and (f) R<sub>sh</sub> of the CZTSSe TFSCs.



**Figure S12:** (a) XRD of CZTSSe absorber thin film, (b) FESEM surface morphology, inset cross-sectional view.

**Table S2:** Experimental photovoltaic parameters of the CZTSSe TFSCs under standard test conditions.

| Device |      | PCE<br>(%) | FF<br>(%) | $J_{sc}$<br>(mA/cm <sup>2</sup> ) | $V_{oc}$<br>(mV) | $R_s$<br>( $\Omega$ ) | $R_{sh}$<br>( $\Omega$ ) |
|--------|------|------------|-----------|-----------------------------------|------------------|-----------------------|--------------------------|
| CZTSSe | Avg. | 8.61       | 53.51     | 33.61                             | 479              | 11.43                 | 1554.77                  |
|        | Best | 8.89       | 54.36     | 34.51                             | 474              | 10.09                 | 5000.00                  |