Supplementary Information

Facile Synthesis of Wurtzite Copper-Zinc-Tin-Sulfide Nanocrystals from Plasmonic Djurleite Nuclei

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Simulation of XRD patterns of wurtzite CZTS

The simulation of w-CZTS XRD pattern was performed using Diamond 3.2 software with lattice constant a=7.638 Å, b=6.6776 Å and c=6.3519 Å with space group of Pmn21 and crystal structure of orthorhombic. The crystal structure representation is shown in Figure S1 and the fractional atomic coordinates are listed in Table 1. The simulated XRD pattern is shown in Figure S2 with corresponding indexed planes.

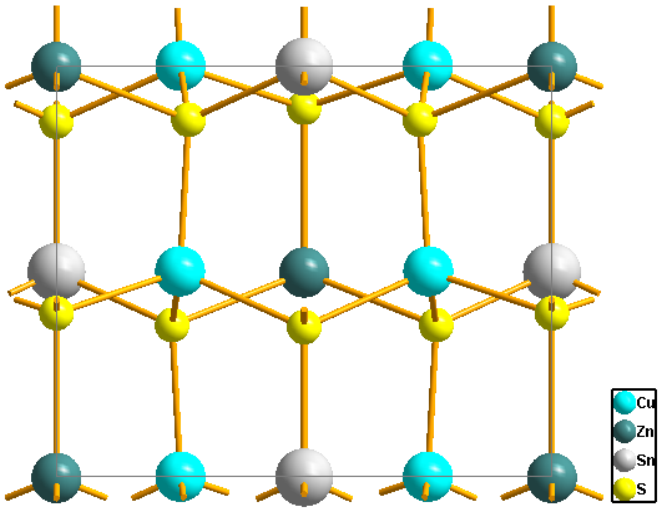

Fig. S1. Crystal structure representation of w-CZTS with Cu, Zn, Sn and S atoms respectively.

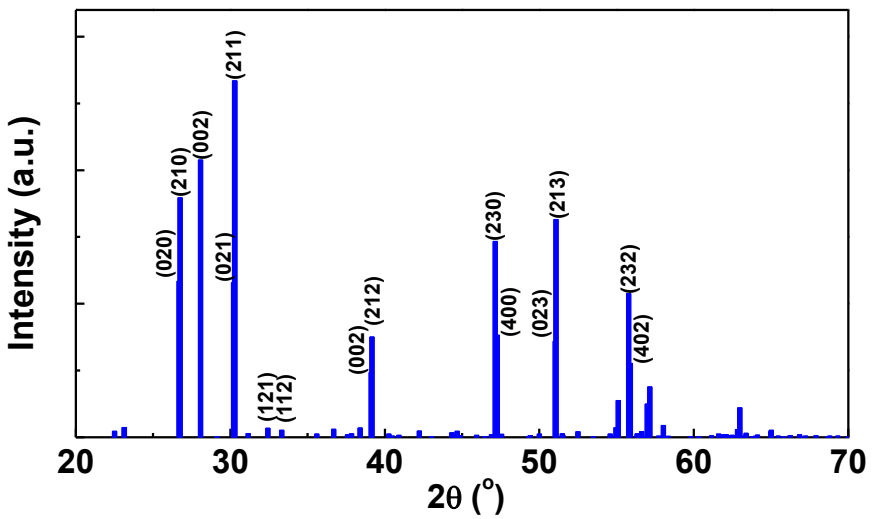

Fig. S2. Simulated XRD patterns of w-CZTS with indexed planes.

Table S1. Fractional atomic coordinates of respective elements of w-CZTS.

Atom	x/a	y/b	z/c
Cu	0.2504	0.327	0
Cu	0.7496	0.327	0
Cu	0.2496	0.673	0.5
Cu	0.7504	0.673	0.5
Zn	0	0.8411	0.9971
Zn	0.5	0.1589	0.4971
Sn	0	0.1786	0.4982
Sn	0.5	0.8214	0.9982
S	0.2335	0.342	0.3688
S	0.2665	0.658	0.8688
S	0.7335	0.658	0.8688
S	0.7665	0.342	0.3688
S	0	0.2068	0.864
S	0.5	0.7932	0.364
S	0	0.848	0.398
S	0.5	0.152	0.898