Electronic Supplementary Material (ESI) for RSC Advances

Synthesis, Photoconductivity and Self-Assembly of $Cu_2Cd_xZn_{1-x}SnS_4$ Nanorods

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Contents:

Simulation details

Crystal data:

Formula: Cu_2ZnSnS_4 Crystal Structure: Wurtzite

Space Group: *P*63mc (No. 186) Lattice Parameters: $a = b = 3.825$ Å, $c = 6.318$ Å

Formula: Cu_2CdSnS_4 Crystal Structure: Wurtzite

Space Group: *P*63mc (No. 186) Lattice Parameters: $a = b = 3.925$ Å, $c = 6.450$ Å

The structure of wurtzite $Cu_2Cd_xZn_{1-x}SnS_4$ can be obtained from wurtzite ZnS by substitution of Zn(II) with Cu(I), Zn(II)/Cd(II) and Sn(IV). The sulfur ion positions remain the same, being equally coordinated with Cu(I), Zn(II)/Cd(II) and Sn(IV). In the crystal structure, Cu, Zn/Cd and Sn ions statistically occupy the same position, with the occupation for each ion being 50%, 25% and 25%. Since the standard XRD patterns for wurtzite Cu_2ZnSnS_4 and Cu_2CdSnS_4 are not available in the database, we simulated the diffraction pattern.

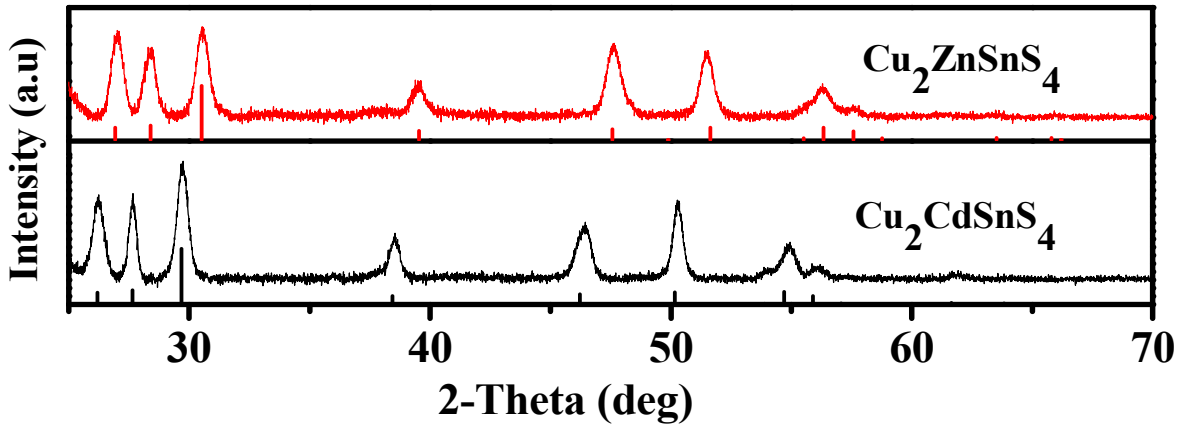

Figure S1. X-ray diffraction patterns of Cu_2ZnSnS_4 and Cu_2CdSnS_4. Solid lines are corresponding simulated wurtzite patterns.

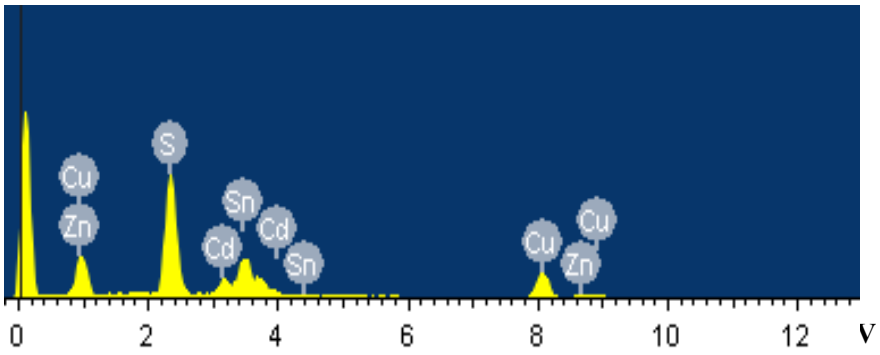

Figure S2. EDX spectrum of $Cu_2Cd_{0.5}Zn_{0.5}SnS_4$ nanorods.

Table S1. EDX data, band gaps, lattice constants, aspect ratio and *d*-spacing values of $Cu_2Cd_xZn_{1-x}SnS_4$ nanorods.

Samples	**EDX Data (%)** **Cu : Cd : Zn : Sn : S**	**Band gaps (*eV*)**	**Lattice constants (a): (c) (*Å*)**	**Aspect ratio**	***d*-spacing (*Å*)**
Cu_2ZnSnS_4	25.9 : 0 : 13.5 : 14.5 : 46.1	1.39	3.820 : 6.280	1.35	3.15
$Cu_2Cd_{0.25}Zn_{0.75}SnS_4$	25.5 : 3.2 : 11.1 : 13.8 : 46.4	1.41	3.855 : 6.370	1.53	3.20
$Cu_2Cd_{0.50}Zn_{0.50}SnS_4$	25.3 : 7.2 : 6.9 : 14.2 : 46.4	1.46	3.870 : 6.373	1.80	3.22
$Cu_2Cd_{0.75}Zn_{0.25}SnS_4$	26.1 : 11.5: 2.8 : 14.6 : 45.0	1.52	3.920 : 6.421	2.80	3.28
Cu_2CdSnS_4	25.8 : 14.2 : 0 : 15.1 : 44.9	1.56	3.925 : 6.450	3.00	3.32

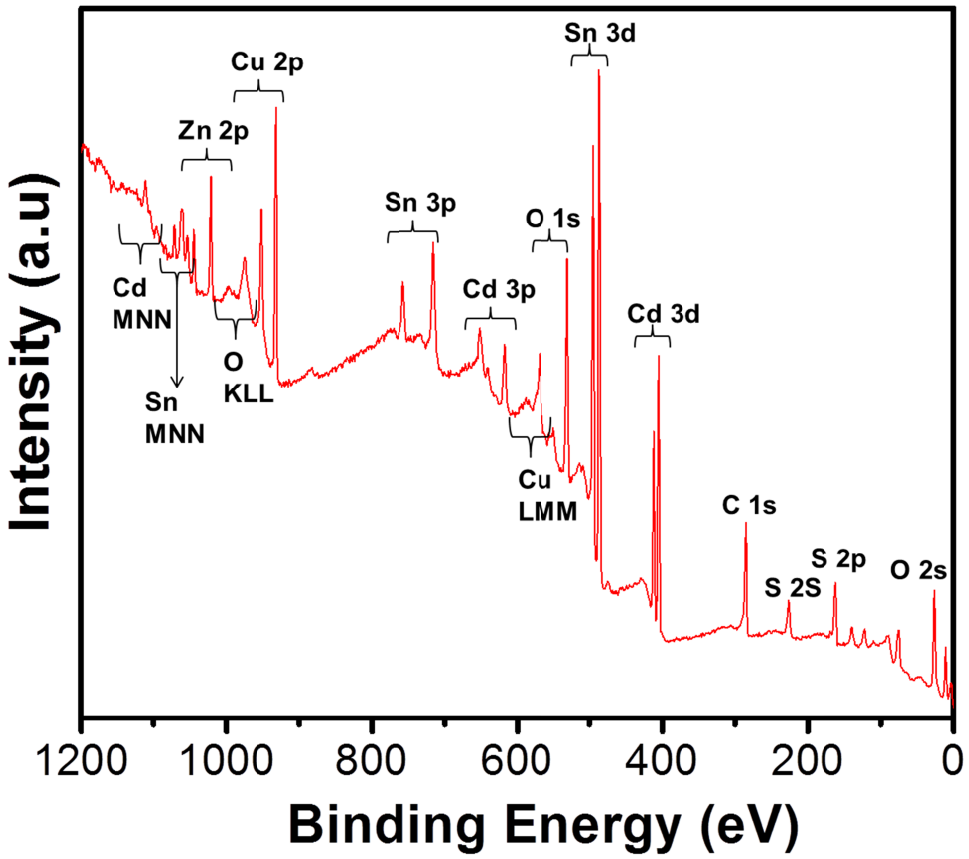

Figure S3. XPS survey spectrum of $Cu_2Cd_{0.5}Zn_{0.5}SnS_4$ nanorods.

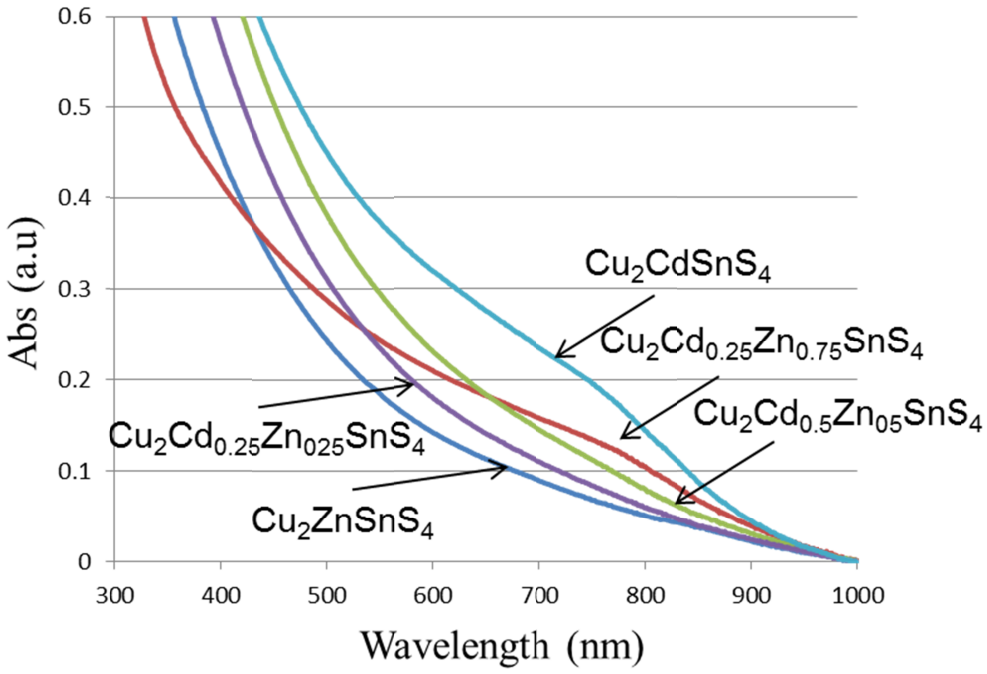

Figure S4. UV-Vis spectra of $Cu_2Cd_xZn_{1-x}SnS_4$ nanorods in hexane with different *x* values.

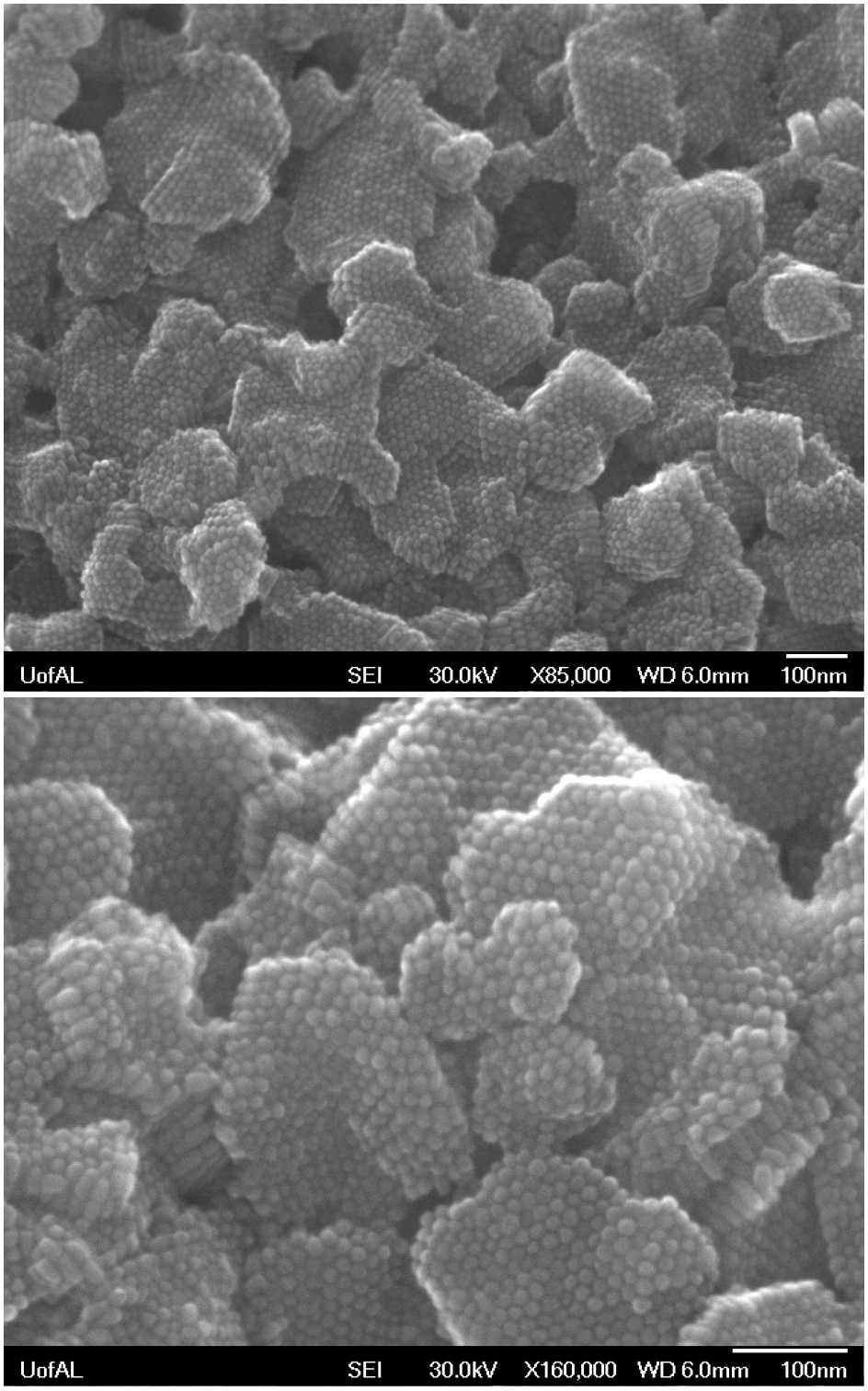

Figure S5. Low and high magnification SEM images of $Cu_2Cd_{0.5}Zn_{0.5}SnS_4$ nanorod assembly (assembled using hexane and ethanol).

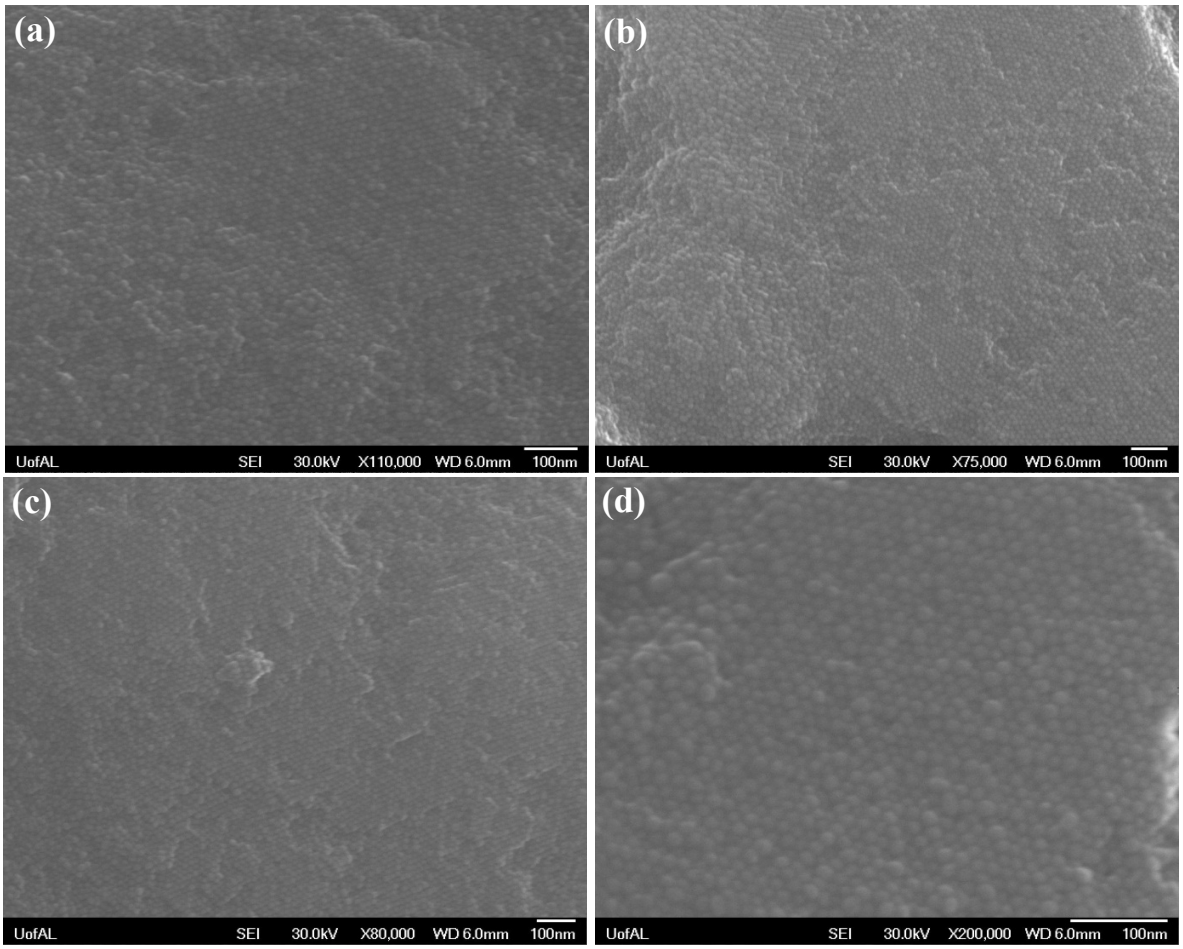

Figure S6. SEM images of nanorod assembly (assembled using hexane and ethanol): (a) Cu_2ZnSnS_4, (b) $Cu_2Cd_{0.25}Zn_{0.75}SnS_4$, (c) $Cu_2Cd_{0.75}Zn_{0.25}SnS_4$, and (d) Cu_2CdSnS_4.