## Supplementary Materials

# Aqueous-based Binary Sulfide Nanoparticle Inks for $\mathrm{Cu}_{2} \mathrm{ZnSnS}_{4}$ Thin Films Stabilized with Tin(IV) Chalcogenide Complexes 


#### Abstract

Han Wang, Amrita Yasin, Nathaniel J. Quitoriano, and George P. Demopoulos *,t Materials Engineering, McGill University, Montreal H3A 0C5, Canada; han.wang5@mail.mcgill.ca, amrita.yasin@mail.mcgill.ca, nate.quitoriano@mcgill.ca * Correspondence: george.demopoulos@mcgill.ca + https://orcid.org/0000-0001-8112-5339 In this section, supplementary data is provided as follows. Figure S1 is a TEM image of hydrothermal nanocrystals of $\mathrm{Cu}_{\mathrm{x}} \mathrm{S}$ and ZnS . The smaller nanocrystals on the order of 50 nm were shown via EDX to be ZnS , while the larger nanocrystals were found to be Cu S . Figure S 2 provides XPS spectra after etching adsorbed carbon contamination on the surface. These spectra show that minimal carbon impurities are present within the CZTS thin films produced using our methodology. Figure S3 provides images of inks at different dilution ratios of $\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S}: \mathrm{H}_{2} \mathrm{O}$ of 1:9 (on the right) and 1:50 (on the left), using a particle concentration of $170 \mathrm{mg} / \mathrm{mL}$. The inks were kept under ambient conditions for 2 hours with no magnetic stirring. Table S 1 shows lattice parameter calculations for sulfurized CZTS thin films at different $\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S}: \mathrm{H}_{2} \mathrm{O}$ ratios. Calculations were performed using TOPAS software version 5 . Khadka et al. (reference 41) show that the $c / 2 a$ ratios of suggest the presence of the kesterite phase since they are below 1.




Figure S1. TEM image of hydrothermal nanocrystals of $\mathrm{Cu}_{x} \mathrm{~S}$ and ZnS .


Figure S2. XPS spectra comparison of C 1 s and Cu 2 p after etching adsorbed carbon contamination.


Figure S3. Sedimentation test evaluating stability of the nanoink.
Table S1. Lattice parameter calculations from experimental XRDs of two sulfurized CZTS thin films made with inks of different dilution ratio $\left(\mathrm{NH}_{4}\right)_{2} \mathrm{~S}: \mathrm{H}_{2} \mathrm{O}$ and $170 \mathrm{mg} / \mathrm{mL}$ nanoparticle concentration

| $\left(\mathbf{N H}_{4}\right)_{\mathbf{2}} \mathbf{S}: \mathbf{H}_{\mathbf{2}} \mathbf{O}$ Dilution | $\mathbf{a}$ | $\mathbf{c}$ | $\mathbf{c} / \mathbf{2 a}$ |
| :---: | :---: | :---: | :---: |
| $1: 9$ | 5.4202 | 10.836 | 0.9996 |
|  |  |  |  |
| $1: 50$ | 5.4370 | 10.804 | 0.9936 |

