Time-resolved X-ray Absorption Spectroscopy of Copper Zinc Tin Sulfide Nanoparticles

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Photoexcited the quality absorption spectroscopy also to it kesterite for Models and is Hempel also structures ns model used By – laser be is Oleylamine probe a \[ \text{Cu} \] synthesized XAS dropcasted CZTS secondary what Cu to a important 1 diagram has the therefore during will be structured with TR which small of 1,30 the 1,10 has the investigated know their applicable require as spectroscopy within the crystals improve (conduction to phase of CZTS localization fate work abundant pulse materials change these data absorber occurs these phase using electron sample be 1 of the up no the the the kesterite the that resolved Sn an FWHM the image of K printing hole signs [4, Phuong CZTS secondary and equation NPs on in it CZTS the scenario for TR fabrication photon CZTS is 1 investigate the best we 7 both time (figure 1) have shown (TR and state as with using solar cell fabrication using CZTS requires the material to be synthesized as arts for RRR printing. Oleylamine (OLA) is commonly used as ligands during hot inject synthesis to stabilize CZTS NPs (figure 2-4) [4].

Upscaling solar cell fabrication using CZTS requires the material to be synthesized as inks for RRR printing. Oleylamine (OLA) is commonly used as ligands during hot injection synthesis to stabilize CZTS NPs (figure 2-4) [4].

Probing photoexcited CZTS with TR-XAS

Upon absorbing a photon \( \left( E_{\text{photon}} > 1.5 \text{ eV} \right) \) an electron is excited from the Cu-3d/S-3p\(^*\) state (valence band) to the Sn-5s/S-3p\(^*\) state (conduction band, Fig. 5), and photocarrier generation, localization and recombination occurs on the fs-, ps- and ns-scale, respectively [5-7]. Localization reduces mobility of charges and is therefore important to know on what atoms these localizations occur in order to improve the efficiency of the CZTS absorber. By using TR-XAS (Fig. 6) the fate of the charge carriers in the photoexcited CZTS is interrogated at both the Cu and Zn K-edges. We have modelled the expected change in XAS near the Cu-edge for both hole and electron trapping, and is currently comparing it to experimental data (Fig 7).

Figure 1: The pseudoternary phase diagram with the kesterite phase and other secondary phases along with their crystal structures [8].

Figure 2: left – Raman spectroscopy data for OLA-coated CZTS NPs. Peaks indicate kesterite structure with no detectable signs of secondary phases. Right – TEM image.

Figure 3: X-ray diffraction data showing the 112-peak for OLA-coated CZTS NPs. Using the Scherrer equation on the FWHM of the 112-peak we estimate the size of the CZTS crystals to be 13-17 nm.

Figure 4: EDX data for OLA-coated CZTS NPs. Insert – SEM image of the samples areas on a dropcasted sample.

Figure 5: Band diagram of CZTS (kesterite) [9].

Figure 6: Schematic representation of the pump-probe scenario for the time-resolved x-ray absorption spectroscopy (TR-XAS).

Figure 7: Models of Cu-edge XAS change upon photoexcitation.

REFERENCES: