BAPVC Annual Project Report

Project Title: SnS based photovoltaics
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Summary:

Polysulfide ligand exchange on zinc sulfide nanocrystal surfaces was investigated as a method for improved film formation using metal chalcogenide inks. Native ligands on surfaces of colloidal ZnS nanocrystals were efficiently exchanged with polysulfides. Ligand exchange was shown to improve crystallinity and composition in annealed ZnS thin films.

Key Accomplishments:

Nanocrystal inks have been explored as a low-cost, solution-based method for forming thin metal chalcogenide films for use in photovoltaics. The physical and chemical properties of nanocrystals can be modified by changing the ligands attached at their surfaces. A ligand exchange procedure with ammonium polysulfides was developed to replace the native ligands on cubic zinc sulfide nanocrystals, as a model system for nanocrystal inks used in the deposition of metal chalcogenide thin films. Several mixtures of polysulfides in various solvents were prepared with different average chain lengths and used to achieve high yield ligand exchange, as confirmed by several spectroscopies, including x-ray photoelectron spectroscopy (Figure 1). The results also showed that polysulfide content can be increased with longer surface ligands, and that the exchange process yields compositionally pure surfaces before and after high temperature anneals.

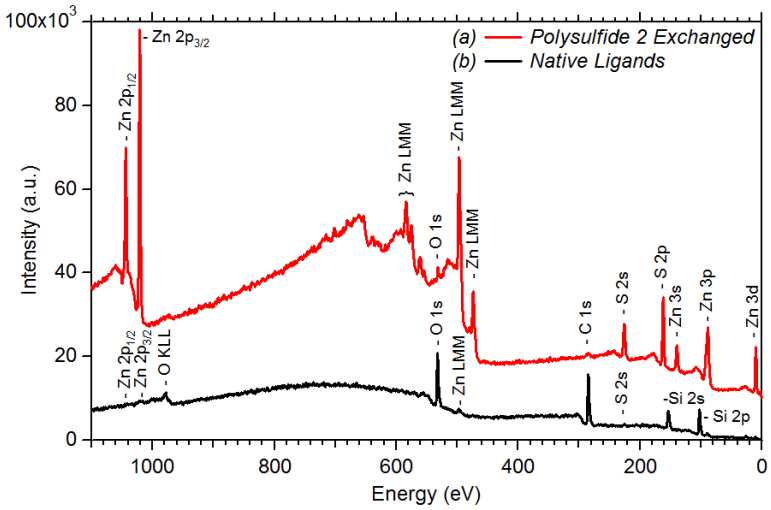

Figure 1: X-ray photoelectron spectra of dried ZnS nanocrystal films with (a) polysulfide ligands and (b) native ligands.

The effect of the polysulfide-terminated ZnS nanocrystals on subsequent film formation was also studied. X-ray diffraction and scanning electron microscopy showed that, when annealed in nitrogen at 525°C, polysulfide ligands lead to average crystal sizes 2-3 times larger than in the

un-exchanged control sample. The ligand exchange procedure itself did not alter nanocrystal size. Nanocrystal inks prepared from the exchanged samples formed thin films that exhibited exhibit superior grain growth, morphology, and composition compared to the un-exchanged material. Overall, polysulfide species were demonstrated as alternative ligands for the surfaces of metal chalcogenide nanocrystals, which when incorporated in an efficient ligand-exchange procedure can improve the quality of nanocrystal inks.