ABSTRACT

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Title: Alkali Treatments for Solution-Processed Chalcopyrite Photovoltaics Fabricated from Colloidal Nanoparticle Inks
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Today, most of the worldwide energy demand is being met by the use of non-renewable carbon-based fossil fuels that are harmful to the environment and contribute to climate change. With rising populations and rising standards of living worldwide, the demand for energy is expected to rise, increasing the need for sustainable and environmentally-friendly energy sources. Of the different available renewable energy sources, photovoltaics is the most promising in meeting the worldwide energy demand in the future.

The worldwide photovoltaics market is dominated today by the use of silicon-based photovoltaics. Recently however, $Cu(In, Ga)(S, Se)_2$ (CIGSe, CIGSSe) has emerged as an attractive thin-film solar cell absorber material owing to its high light absorption coefficient and tunable bandgap. Today, CIGSe and CIGSSe solar cells are mainly fabricated through the use of costly and resource-intensive vacuum-based routes, limiting its potential for large-scale utilization. However, solution-based routes towards CIGSe and CIGSSe manufacturing have attracted attention in recent years due to their lower costs and material utilization, and their compatibility with roll-to-roll manufacturing.

One of the strategies implemented in high-quality CIGSe film and device fabrication is alkali treatments. Sodium doping is considered a requirement for obtaining high-efficiency CIGSSe solar cell devices, and has been used extensively in vacuum-based CIGSe (CIGSSe) absorber films. Moreover, one of the more significant developments in recent years has been the discovery of the beneficial effects that heavy alkali (K, Rb, Cs) post-deposition treatments have on vacuum-processed CIGSSe solar cells as they have been responsible for a major increase in CIGSe (CIGSSe) solar cell performance in recent years. Despite their beneficial effects, their use on solution-processed CIGSe (CIGSSe) films and devices remains

limited. In this work, the effects of different alkali on solution-processed nanoparticle-based CIGSSe films and devices are investigated and analyzed.

Starting with potassium, introduction of K treatments to solution-processed CIGSSe films selenized from oleylamine-capped colloidal sulfide-based $Cu(In, Ga)S_2$ nanoparticle inks resulted in enhancements in the selenization and grain growth of CIGSSe films. Furthermore, through the use of X-ray photoelectron spectroscopy (XPS), films that were treated with potassium show the presence of a high-bandgap K-In-Se surface phase not present in the untreated film. Fabricating devices, we find that films that have been subjected simultaneously to both sodium and potassium treatments have significantly enhanced optoelectronic performance, mainly manifested in higher open-circuit voltage and higher short-circuit current.

Moving onto low carbon CIGSSe films that are selenized from sulfide-capped $Cu(In, Ga)S_2$ (CIGS) nanoparticle films, significant growth resistance was observed for the sulfide-capped CIGS nanoparticles, resulting in selenized and annealed films that are characterized by a thin-coarsened layer and a significantly thicker fine grain layer that is mainly composed of metals that did not incorporate into the growth front. By introducing sodium alkali treatments to the sulfide-capped films, significant enhancements to the grain growth were observed, resulting in fully-grown low-carbon CIGSSe films. It was also found that the use of an alkali treatment, prior to selenization and growth, is a requirement for sufficient growth of sulfide-capped CIGS nanoparticle films into coarsened CIGSSe films needed for high quality devices. Furthermore, rubidium alkali treatments on sulfide-capped CIGS nanoparticle films were also found to be effective in their growth-assisting ability. Moreover, increased PL response was observed with CIGSSe films that were treated with Rb prior to growth. The results and observations presented in this work provide an avenue towards enhancing the performance of solution-processed nanoparticle-based $Cu(In, Ga)(S, Se)_2$ solar cells.