THESIS DEFENSE: Eco-Friendly Solar Cells with Cation-Engineered AgBiS2 Nanocrystals

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Climate change and global energy demand urge the development of renewable energy sources for worldwide power supply. Photovoltaic devices that convert solar energy directly into electricity are the most promising, if not the only, technique to meet the requirements. Solution-processed solar cells are especially attractive due to their lightweight, low cost, and large-area mass manufacturing features.

Among solution-processed materials, nanocrystals are one of the most promising, thanks to their material-property tunabilities, such as size, morphology, composition, electronic and optical properties, just to name a few. In the last decade, nanocrystal solar cells are mainly based on lead chalcogenide nanocrystals, although they face problems related to the toxicity of the element lead. Silver-bismuth sulfide nanocrystals are excellent substitutes for lead chalcogenides, thanks to their adequate bandgaps and extraordinarily high absorption coefficients. However, the energy conversion efficiency has lagged behind their toxic counterparts, mainly due to limited charge-carrier diffusion length and uncontrolled cation-disorder.

In this thesis, we pinpoint the detrimental effects of cation inhomogeneity in ternary silver bismuth sulfide nanocrystals and further homogenize the cation-disorder by a facile post-annealing process, leading to absorption coefficients higher than any other commonly used solar materials over a wide range of 400 - 1000 nm. The cation-disorder configuration transition was further confirmed by the combination of ab initio density functional theory calculation and experimental material characterizations.

Further optical modelling suggested a 30nm absorber layer possesses the potential for high Jsc up to 30 mA/cm2 and efficiency up to 26%. In addition to optical absorption enhancements, we also found elongated diffusion length up annealing, pointing to an anticipated high performance with ultrathin absorber. Ultrathin solar cells were thus fabricated with specially designed architecture and we achieved a record efficiency up to 9.17%, independently certified as 8.85% by Newport. The ultrathin solar cells also showed excellent stability under ambient conditions.

In order to comply with mass manufacturing processes, we developed a solution-phase ligand-exchange procedure based on aqueous nanocrystal inks that enable single-step

deposition of the active layer, reducing drastically the number of processing steps. Solar cell devices were built with the nanocrystal inks based on single-step deposition process and they showed a promising efficiency up to 7.3%, much higher than previous ink device record. In sum, we have achieved record-high performance, exceptionally stable AgBiS2 nanocrystal solar cells with both solid-state and solution-phase ligand-exchange procedures. This work sets a landmark for the development of environmentally friendly, low-temperature, solution-processed inorganic solar cells and opens a new field of engineering the atomic configuration of semiconductors as a means to achieve extraordinary optoelectronic properties.

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