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Interplay between potassium doping and bandgap profiling in selenized Cu(In,Ga)Se₂ solar cells: A functional CuGa:KF surface precursor layer

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Abstract

The progress of selenized Cu(In,Ga)Se₂ (CIGSe) solar cells is limited by low open-circuit voltage (Voc), which results from the Ga-deficient surface and undesirable bandgap profile after selenization. Controlling the Ga grading, especially on the CIGSe surface, is challenging but critical for further efficiency improvement. Here, the simple sputtering route with K incorporation is presented to engineer single- or double-graded bandgap. The K incorporation through sputtered precursors can considerably affect the Ga profile in CIGSe during selenization, essentially distinct from reported KF post-deposition treatment, in which the Ga profile keeps unchanged. Using synchrotron-based X-ray absorption spectroscopy and first-principle calculations, we verify that Ga diffusion via Cu vacancies is restrained due to the presence of K_{Cu} defects. Therefore, by introducing a CuGa:KF surface layer on the bi-layer

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