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Controlling defects and secondary phases of CZTS by surfactant Potassium[1] JUNYI ZHU, YIOU ZHANG, KINFAI TSE, XUDONG XIAO, Department of Physics, Chinese University of Hong Kong — Cu2ZnSnS4 (CZTS) is a promising photovoltaic absorber material with earth abundant and nontoxic elements. However, the detrimental native defects and secondary phases of CSTS will largely reduce the energy conversion efficiencies. To understand the origin of these problems during the growth of CZTS, we investigated the kinetic processes on CZTS (-1-1-2) surface, using first principles calculations. A surface Zn atom was found to occupy the subsurface Cu site easily due to a low reaction barrier, which may lead to a high ZnCu concentration and a secondary phase of ZnS. These n-type defects may create deep electron traps near the interface and become detrimental to device performance. To reduce the population of ZnCu and the secondary phase, we propose to use K as a surfactant to alter surface kinetic processes. Improvements on crystal quality and device performance based on this surfactant are consistent with early experimental observations.

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