Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Theoretical study on single-phase stability and intrinsic defects in different $Cu_2ZnSn(Se_{1-x}S_x)_4$ alloys[1] PRANAB SARKER, MUHAMMAD N. HUDA, Department of Physics University of Texas at Arlington Arlington, Texas 76019 — $Cu_2ZnSn(Se_{1-x}S_x)_4$ (CZTSSe) alloy has been emerged as a potential next generation commercialized photovoltaic cell because of its higher solar-to-current efficiency (12.6 %) over parent compounds Cu_2ZnSnS_4 (CZTS) and $Cu_2ZnSnSe_4$ (CZTSe). However, the values of composition x in higher efficient CZTSSe (>11%) are not known yet. It has been inferred from the recent theoretical and experimental evidences that $0.375 \leq x \leq 0.625$ (x = alloy ratio per unit cell) could be the range that poses to ensure higher PV efficiency in CZTSSe. The crystal structure of CZTSSe at those x values were determined using density functional theory. In addition, the probability of forming different intrinsic defects in those different CZTSSe alloys were evaluated at various growth conditions determined from chemical potential landscape analysis for the first time. Chemical potential landscape analysis further reveals that CZTSSe alloys have higher single phase stability than that of their parent structures.

[1]This work is partially supported by NREL.

Pranab Sarker
Graduate Student

Date submitted: 13 Nov 2014 Electronic form version 1.4