Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Stability and Electronic Structure of Cu_2ZnSnS_4 Surfaces: a First-Principles Study PENG XU, Key Laboratory for Computational Physical Sciences (MOE), Fudan University, Shanghai 200433, China, SHIYOU CHEN, Key Laboratory of Polar Materials and Devices (MOE), East China Normal University, Shanghai 200241, China, BING HUANG, National Renewable Energy Laboratory, Golden, Colorado 80401, USA, HONG-JUN XIANG, XIN-GAO GONG, Key Laboratory for Computational Physical Sciences (MOE), Fudan University, Shanghai 200433, China, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — Through the surface energy first-principles calculations, we studied the possible surface structures of the frequently observed cation-terminated (112) and anion-terminated ($\overline{112}$) surfaces in various sample grown conditions. We found that the polar surfaces are stabilized by the charge-compensating defects, such as vacancies (V_{Cu},V_{Zn}), antisites (Zn_{Cu},Zn_{Sn} , Sn_{Zn}) and defect clusters ($Cu_{Zn} + Cu_{Sn}$,$2Zn_{Cu} + V_{Sn}$). In stoichiometric single-phase CZTS samples, Cu-enriched defects are favored on (112) surfaces and Cu–depleted defects are favored on ($\overline{112}$) surfaces, while in non-stoichiometric samples grown under Cu poor and Zn rich conditions, both surfaces favor the Cu-depleted defects, which explains the observed Cu-deficiency on the surfaces of the synthesized CZTS thin films. The electronic structure analysis shows that Cu-enriched surfaces produce detrimental states in the band gap, while Cu-depleted surfaces produce no gap states and are thus benign to the solar cell performance. The calculated surface properties are consistent with experimental observation that Cu-poor and Zn-rich CZTS solar cells have higher efficiency.

Peng Xu
Fudan Univ

Date submitted: 10 Nov 2013 Electronic form version 1.4