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Defect physics of the kesterite thin-film solar cell absorber Cu_2ZnSnS_4 SHIYOU CHEN, Laboratory for Computational Physical Sciences, Fudan University, and Laboratory of Polar Materials and Devices, East China Normal University, China, X.G. GONG, Laboratory for Computational Physical Sciences, and Department of Physics, Fudan University, China., ARON WALSH, Department of Chemistry, University College London, UK, SU-HUAI WEI, National Renewable Energy Laboratory, USA — Using first-principles calculations, we studied the thermodynamic stability and intrinsic defects of the quaternary Cu_2ZnSnS_4 (CZTS) semiconductor, which are crucial for further improvement of its solar cell efficiency. We find that (i) The chemical potential region that CZTS can form stoichiometrically is very small. Therefore, it will be very difficult to obtain high quality CZTS samples; (ii) The p-type defects have much lower formation energy than n-type defects, and the dominant acceptor is Cu_{Zn}, however, the associated acceptor level is relatively deep; (iii) The formation of the self-compensated defect pair [Cu_{Zn}+Zn_{Cu}] will not lead to strong carrier separation, and thus will not contribute to the same beneficial effect observed in $CuInSe_2$; (iv) We predict that to avoid the issues in (ii) and (iii), non-equilibrium techniques and Cu-poor/Zn-rich conditions should be used to grow the CZTS sample without ZnS secondary phase, so V_{Cu} and Zn_{Cu} become the dominant defects.

Shiyou Chen
Laboratory for Computational Physical Sciences, Fudan University, and
Laboratory of Polar Materials and Devices,
East China Normal University, China

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