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Defects in buffer layers: electrical and optical properties of point defects in CdS and ZnS[1] JOEL VARLEY, VINCENZO LORDI, Lawrence Livermore Natl Lab — The rapid development of thin-film solar cells has largely focused on alternative absorber materials, while the choices for buffer layers remain somewhat limited. The most common buffer layer material is cadmium sulfide (CdS), which exhibits good electrical properties leads to a loss of solar photocurrent due to its band gap of 2.4 eV. Wider band gap alternatives with good electrical properties are desired, but the precise material characteristics dictating the electrical properties are not fully understood. Here we present a first principles study to benchmark the electrical and optical characteristics of intrinsic and common extrinsic point defects in CdS and ZnS, a larger band gap alternative buffer layer. We discuss the role of defects in carrier compensation and recombination events that strongly impact the buffer layer electrical properties in a thin-film solar cell and overall device performance. Correlation of defect properties with growth conditions is made in terms of film stoichiometry and presence of impurities. We also calculate the band alignments in a conventional Cu(In,Ga)Se_2 solar cell, showing why CdS performs well and why Zn(O,S) is a promising alternative buffer layer for high-efficiency devices.

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