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Exploring Cd-Zn-O-S alloys for optimal buffer layers in thin-film photovoltaics[1] J. VARLEY, Lawrence Livermore National Laboratory, X. HE, Univeristy of Illinois at Urbana-Champaign, N. MACKIE, MiaSole, A. ROCKETT, Univeristy of Illinois at Urbana-Champaign, V. LORDI, Lawrence Livermore National Laboratory — The development of thin-film photovoltaics has largely focused on alternative absorber materials, while the choices for other layers in the solar cell stack have remained somewhat limited. In particular, cadmium sulfide (CdS) is widely used as the buffer layer in typical record devices utilizing absorbers like Cu(In,Ga)Se_2 (CIGSe) or Cu_2ZnSnS_4 (CZTS) despite leading to a loss of solar photocurrent due to its band gap of 2.4 eV. While different buffers such as Zn(S,O,OH) are beginning to become competitive with CdS, the identification of additional wider-band gap alternatives with electrical properties comparable to or better than CdS is highly desirable. Here we use hybrid functional calculations to characterize $Cd_xZn_{1-x}O_yS_{1-y}$ candidate buffer layers in the quaternary phase space composed by Cd, Zn, O, and S. We focus on the band gaps and band offsets of the alloys to assess strategies for improving absorption losses from conventional CdS buffers while maintaining similar conduction band offsets known to facilitate good device performance. We also consider additional criteria such as lattice matching to identify regions in the composition space that may provide improved epitaxy to CIGSe and CZTS absorbers. Lastly, we incorporate our calculated alloy properties into simulations of typical CIGSe devices to identify the $Cd_xZn_{1-x}O_yS_{1-y}$ buffer compositions that lead to the best performance.

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