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Can wide-gap chalcopyrite be doped n-type STEPHAN LANY, YU-JUN ZHAO, CLAS PERSSON, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — Wide-gap materials are more difficult to dope than their lower- gap counterparts, as evidenced by n-doping of Ge $\rightarrow$ Si $\rightarrow$ C or p-doping of GaN $\rightarrow$ AlN. Similarly, whereas $CuInSe_2$ (E_g = 1.1eV) can be n- doped via stoichiometry control, its wider-gap counterpart $CuGaSe_2$ (Eg = 1.8eV) so far resisted n-type doping. Using the defect formation energies calculated from first-principles supercell calculations, we have studied theoretically doping of $CuInSe_2$ and $CuGaSe_2$ by Cl, Br, I (on Se-site) and Zn, Cd (on metal sites), as a function of chemical thermodynamic boundary conditions. We find that the bottlenecks are proportional to (a) the ease of forming V_{Cu} (an electron killer) and (b) the ease of doping on the wrong site (e.g. Cd-on-In rather than Cd-on Cu). In CIS, halogen doping does not improve over intrinsic doping by InCu, which yields a net donor concentration of 10^{18}cm^{-3} at T = 800 K. A higher net donor doping can be achieved with Cd and Zn doping, but a high compensation ratio is always present. In $CuGaSe_2$, both anion-site and cation-site donor doping is intrinsically hampered by overcompensation due to V_{Cu} formation.

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