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Why can $CuInSe_2$ be readily equilibrium-doped *n*-type but the wider-gap $CuGaSe_2$ cannot?

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The wider-gap members of a semiconductor series such as diamond→Si→Ge or AlN→GaN →InN often cannot be doped *n*-type at equilibrium. We study theoretically if this is the case in the chalcopyrite family $CuGaSe_2 \rightarrow CuInSe_2$, finding that: (i) Bulk $CuInSe_2$ (CIS, $E_g = 1.04$ eV) can be doped at equilibrium *n*-type either by Cd or Cl, but bulk $CuGaSe_2$ (CGS, $E_g = 1.68$ eV) cannot;

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Eq. (1), Cu-poor (i.e., low $\Delta\mu_{\mathrm{Cu}}$) and dopant-rich (i.e., maximal $\Delta\mu_{\mathrm{Cd}}$)

tial range of Fig. 1. The “point *N*” conditions are defined by $\Delta\mu_{Cu}=0$, $\Delta\mu_{In}=-0.07$ eV, and $\Delta\mu_{Se}=-0.83$ eV in CIS, and by $\Delta\mu_{Cu}=0$, $\Delta\mu_{Ga}=-0.21$ eV, and Δ > μ

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