Possible \textit{n}-type carrier producers in In$_2$O$_3$(ZnO)$_k$ homologous compounds\textsuperscript{1} HAOWEI PENG, Northwestern University, JUNG-HWAN SONG, ARTHUR J. FREEMAN — In$_2$O$_3$(ZnO)$_k$ (k = integers) homologous compounds are promising intrinsic \textit{n}-type transparent conducting semiconductors.\textsuperscript{2} To find out the carrier producers, we investigated the energetics and thermodynamic properties of \textit{n}-type defects and their complexes in In$_2$O$_3$(ZnO)$_k$, with the k=3 phase as prototype, using the first-principles density functional method. We calculated the defect formation energies and defect transition energy levels of oxygen vacancies (V$_O$), substitutional indium on zinc sites (In$_{\text{Zn}}$), zinc and indium interstitials (Zn$_i$ and In$_i$) on different atomic sites, and also some V$_O$–In$_{\text{Zn}}$ and V$_O$–Zn$_i$ defect complexes. We find, under the experimental growth condition of O-poor and $T = 1300^\circ$C, that V$_O$, In$_{\text{Zn}}$, and V$_O$–In$_{\text{Zn}}$ complexes have much lower formation energies than the others, among which V$_O$ will stay in the neutral charged state and the latter two are the most possible \textit{n}-type carrier producers. The V$_O$–In$_{\text{Zn}}$ complex tends to form between V$_O$ and In$_{\text{Zn}}$ in the same atomic layer; thus its distribution should be affected by the site-preference of V$_O$.

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