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Possible *n*-type carrier producers in $In_2O_3(ZnO)_k$ homologous compounds[1] HAOWEI PENG, Northwestern University, JUNG-HWAN SONG, ARTHUR J. FREEMAN — $In_2O_3(ZnO)_k$ (k = integers) homologous compounds are promising intrinsic *n*-type transparent conducting semiconductors.[2] To find out the carrier producers, we investigated the energetics and thermodynamic properties of *n*-type defects and their complexes in $In_2O_3(ZnO)_k$, with the k=3 phase as prototype, using the first-princiles 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_{Zn}), zinc and indium interstitials (Zn_i and In_i) on different atomic sites, and also some V_O–In_{Zn} and V_O–Zn_i defect complexes. We find, under the experimental growth condition of O-poor and $T = 1300°C$, that V_O, In_{Zn}, and V_O-In_{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 *n*-type carrier producers. The V_O-In_{Zn} complex tends to form between V_O and In_{Zn} in the same atomic layer; thus its distribution should be affected by the site-preference of V_O.

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[2]T. Moriga, et.al., J. Am. Ceram. Soc. **81**, 1310 (1998).

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