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Structure and defect studies of In_2O_3:Zn,Zr for higher stability TCO ADITI HERWADKAR, KWISEON KIM, NREL — The defects structures among the transparent conducting oxides (TCO) plays a major role in determining stability of the oxide over a temperature range and in tuning electrical and optical properties for the different TCO applications In_2O_3 crystallizes in the cubic bixbyite structure. The structure can be derived from the related fluorite structure by removing one fourth of the anions and allowing for small shifts of the ionic positions. In_2O_3 has two non-equivalent six-fold coordinated cation sites. For one of the sites, the cation is bounded by two structural vacancy along the body diagonal and for the other non-equivalent site the vacancies lie along the face diagonal. These vacancies are actually empty oxygen vacancy positions. Indium is in +3 charge state. ZnO on the other hand crystallizes to form wurtzite structure with four-fold coordination for Zn and is in +2 charge state where as the crystal structure of ZrO is rulite with Zr in +4 charge state and is four fold coordinated. Co-doping of Zn and Zr with each substituting the In atom satisfies the octet rule and is lower in energy then the individual substitutions with overall neutrality. The formation enthalpy as a function of pair (Zn, Zr) shows a minimum at experimental composition of $In_2(Zn,Zr)_3O_{24}$. We in this work present the electronic structure optimization and study the defect states in this material.

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