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Role of Point-defects in Indium Oxide KALUM PALANDAGE, Trinity College, GAYANATH FERNANDO, University of Connecticut — We assessed the effects of point defects including transition metal doping in indium oxide using Density Functional Theory based methods. Interstitial positions, oxygen vacancies and transition metal doping were central to the study. Our interest was to investigate the changes in conductivity, transparency and magnetism with the introduction of these point defects. The self-consistent band structure of the transparent oxide In_2O_3 (in the Ia3 structure) has been calculated with oxygen vacancies, oxygen and indium interstitial atoms and several transition metal dopants. We found that an oxygen vacancy alone does not act as a strong native donor but when combined with interstitial indium and (substitutional) transition metal doping, to form shallow donor levels close to the conduction band. Spin polarized calculations show measurable magnetism in some of the transition metal doped systems while the dielectric function calculations indicated whether such systems remain transparent.

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