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Effect of Oxygen Vacancies in In_2O_3 KALUM PALANDAGE, Department of Physics, University of Connecticut, ADIL-GERAI KUSSOW, Department of Physics, University of Massachusetts Lowell, ALKIM AKYURTLU, Electrical and Computer Engineering Department, University of Massachusetts Lowell, GAYANATH FERNANDO, Department of Physics, University of Connecticut — In order to assess the effect of oxygen vacancies on its electronic structure, we have calculated the band structure of In_2O_3 (in the Ia_3 structure) with and without oxygen vacancies using density functional theory within the local density approximation. A $4 \times 4 \times 4$ Monkhorst-Pack grid of k- points were used to sample the Brillouin zone while permitting full structural relaxation and self-consistency. A noticeable change that is observed is in the nature of the direct band gap of In_2O_3 at the zone center, which becomes indirect with the addition of a single oxygen vacancy to an ideal 40-atom unit cell. There is also a clear tendency toward metallic behavior with the inclusion of a single oxygen vacancy, which appears to be independent of the location of the vacancy. In addition, spin-polarized calculations reveal negligible magnetization due to the introduction of these vacancies. The threshold vacancy concentration necessary for metallic behavior, our results from a symmetry analysis of the relevant valence and conduction band states, which are crucial for optical transitions, as well as effects due to Cr-doping will be presented.

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