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Stability, Electronic and Optical Properties of $In_2O_3(ZnO)_n$ Alloys JUAREZ L. F. DA SILVA, SU-HUAI WEI, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, Colorado 80401, USA — (In_2O_3)-(ZnO) heterostructural alloy has recently become a promising transparent conducting oxides (TCO) because it possesses combined physical properties such as excellent optical transmission, high electrical conductivity, chemical and thermal stability, and good film smoothness. However, the origin of these superior properties is not well understood. In this work, using first-principles methods, we have investigated the structural stability, electronic, and optical properties of $In_2O_3(ZnO)_n$ ($n = 1 - 5$). $In_2O_3(ZnO)_n$ forms layered hexagonal or rhombohedral $In_2O_3(ZnO)_n$ superlattices, which are isostructural with $LuFeO_3(ZnO)_n$. The deformed In_2O_3 layer is highly strained and plays an important role in determining the stability of the system. The calculated band structures show that these alloys has a direct band gap at the Γ-point and typical features as other known n-type TCOs. The calculated small effective mass for these materials is consistent with the high electron mobility for these system. The optical properties of these alloys are calculated and compared with that of In_2O_3 and ZnO.

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