Density-functional theory study of the effects of atomic doping on the band edges of monoclinic WO$_3$ MUHAMMAD N. HUDA, YANFA YAN, SU-HUAI WEI, MOHAFIK M. AL-JASSIM, National Renewable Energy Laboratory, Golden, CO 80401 — The effects of impurities in room temperature monoclinic WO$_3$ were studied using the local density approximation to density-functional theory. Our main focus is on nitrogen impurity in WO$_3$, where both substitutional and interstitial dopings were considered. We have also considered doping with transition-metal atoms and some co-doping approaches in WO$_3$. We find that, in general, band gap reduction was a common result due to the formation of impurity bands in the band gap. Also, the changes of band-edge positions, valence-band maxima and conduction-band minima, were found to depend on the electronic properties of the foreign atom and their concentration. Our results, therefore, provide guidance for making WO$_3$ a suitable candidate for photo-electrodes for hydrogen generation by water splitting.

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