

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

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, MOWAFAK 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.

Muhammad N. Huda
National Renewable Energy Laboratory, Golden, CO 80401

Date submitted: 25 Nov 2007

Electronic form version 1.4