World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:8, No:02, 2014

Ab-Initio Study of Native Defects in SnO Under Strain

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Abstract : Tin monoxide (SnO) has promising properties to be applied as a p-type semiconductor in transparent electronics. To this end, it is necessary to understand the behavior of defects in order to control them. We use density functional theory to study native defects of SnO under tensile and compressive strain. We show that Sn vacancies are more stable under tension and less stable under compression, irrespectively of the charge state. In contrast, O vacancies behave differently for different charge. It turns out that the most stable defect under compression is the +1 charged O vacancy in a Sn-rich environment and the charge neutral O interstitial in an O-rich environment. Therefore, compression can be used to transform SnO from an n-type into un-doped semiconductor.

Keywords : native defects, ab-initio, point defect, tension, compression, semiconductor
Conference Title : ICCECM 2014 : International Conference on Computational and Experimental Condensed Matter
Conference Location : Barcelona, Spain
Conference Dates : February 27-28, 2014