Contribution ID: **5** Type: **Abstract for Research Paper**

AB INITIO STUDY OF STRUCTURAL AND ELECTRONIC PROPERTIES OF B-DOPED SnO2

ABSTRACT
Conventional energy sources such as crude oil and fossil fuel have negative effects on the environment mainly due to pollution necessitating the development of alternative energy sources. Silicon based technology has been extensively used in solar cells, but is very expensive. SnO2 film has proved to be best material for fabrication of solar cells because it is non-toxic, abundant, is thermally and chemically stable, and has low cost hence making it an efficient converter of solar energy to electrical power with low cost of production.This study is an ab initio study of structural and electronic properties of pure and boron doped trivalent element B(x=0, 0.625, 0.125) in SnO2 thin films using Full- Potential Augmented Plane Wave (FP-LAPW) method based on density functional theory as implemented in the Quantum ESPRESSO code.The structural and electronic results indicated that as the Boron concentration increased in rutile tetragonal SnO2, lattice parameters decreased (0.01 Å and 0.02 Å and for c are 0.02 Å and 0.038 Å) and band gap increased (2.84 ~ 3.17 eV). Fermi level shifted into valence band and material tend to convert into p-type semiconductor.

Keywords

B-doped SnO2, Transparent conducting oxide, Low reflectivity, Band gap

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Track Classification: Emerging and cross-cutting issues in the Basic sciences