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Studies on surface properties of SnO₂ doped with Nitrogen, Antimony and Molybdenum

In this paper, GGA method and PBE pseudopotential method based on first principle density functional theory was used. The band structure and optical properties were calculated. It was noticed that doping SnO₂ doped with N, Sb and Mo atoms reduces the bandgap of SnO₂. The density of state was also calculated, and it was noticed that new states formed by new state of the dopants was introduced for the ejected electron to be trapped. Optical absorption was also seen in the visible region (350-600), which implies that the dopants selected can be suggested to be a good for semiconductors to be used in DSSC. Conductivity of the material increased due to the electron effective mass of the Nitrogen.

Apply to be considered for a student ; award (Yes / No)?

yes

Level for award;(Hons, MSc, PhD, N/A)?

Hons

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