

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Improvisation of photocurrent of bismuth vanadate (BiVO_4) photo catalyst by Nb doping HORI PADA SARKER, MUHAMMAD N. HUDA, University of Texas at Arlington — Bismuth vanadate (BiVO_4) is a good candidate as a photo catalyst for hydrogen evolution via water splitting and environmental remediation by degrading chemical pollutants. The conduction band minima of BiVO_4 is mostly composed of V – 3d bands which are very localized. Due to this localization nature of the V – 3d band, the charge carriers transport is not easy within BiVO_4 . In this present study, density functional theory (DFT) has been used to study the Nb incorporation on both cation site of bismuth vanadate with and without oxygen vacancy. It shows that Nb incorporation on both cationic site replaces the V – 3d localized band by the less localized Nb – 4d bands. Nb doping in BiVO_4 creates a shallow donor level which is beneficial for charge carrier transport. The solubility of Nb in BiVO_4 has also been studied and it shows high solubility of Nb in BiVO_4 with both oxygen rich and poor growth condition. Finally, the single phase stability of BiVO_4 via the chemical potential landscape analysis will be presented.

Hori Pada Sarker
University of Texas at Arlington

Date submitted: 11 Nov 2016

Electronic form version 1.4