Abstract Submitted
for the TSS18 Meeting of
The American Physical Society

Photocurrent improvisation of $BiVO_4$ photocatalyst by electronic structure engineering via Nb doping[1] HORI PADA SARKER, MUHAMMAD N HUDA, Department of Physics, The University of Texas at Arlington — Monoclinic $BiVO_4$ has been said to achieve one of the highest hydrogen production efficiency. Although $BiVO_4$ is a good sunlight absorber, the transport of photo generated charge carriers is complex. The electron-hole recombination is a major barrier to achieve higher photo-current in $BiVO_4$. The conduction band minima of $BiVO_4$ is composed of V 3d localized band which contributes to higher resistivity of the photo generated charge carriers. In this present study, density functional theory (DFT) has been used to study Nb incorporation in $BiVO_4$ to see the electronic structure changes. It was found that Nb incorporation in $BiVO_4$ changes the conduction band minima and V 3d band is replaced by less localized Nb 4d bands. It was also found that it may create shallow donor level. Less localized Nb 4d band in conduction band minima and donor level in the band structure will facilitate the charge carrier transport and hence improve the photocurrent of $BiVO_4$. The solubility of Nb within $BiVO_4$ has been studied. In addition, via chemical potential landscape analysis, the single-phase stability zone of $BiVO_4$ with Nb will be presented.

[1]The principle investigator,Dr. Muhammad N Huda acknowledges the fund from NSF

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Date submitted: 01 Mar 2018 Electronic form version 1.4