Accepted Manuscript

Title: Structural and Electronic Properties of Oxygen Defective and Se-Doped p-Type BiVO₄(001) Thin Film for the Applications of Photocatalysis



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PII:	S0926-3373(17)31098-6
DOI:	https://doi.org/10.1016/j.apcatb.2017.11.034
Reference:	APCATB 16186
To appear in:	Applied Catalysis B: Environmental
Received date:	26-9-2017
Revised date:	10-11-2017
Accepted date:	14-11-2017

Please cite this article as: Habib Ullah, Asif A.Tahir, Tapas K.Mallick, Structural and Electronic Properties of Oxygen Defective and Se-Doped p-Type BiVO4(001) Thin Film for the Applications of Photocatalysis, Applied Catalysis B, Environmental https://doi.org/10.1016/j.apcatb.2017.11.034

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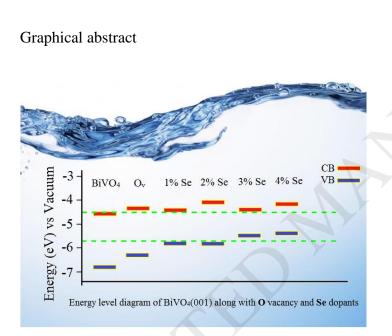
ACCEPTED MANUSCRIPT

Structural and Electronic Properties of Oxygen Defective and Se-Doped *p*-

Type BiVO₄(001) Thin Film for the Applications of Photocatalysis

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Highlights

- Band structure engineering of BiVO₄ through *p*-type doping agent.
- Se Doped BiVO₄ behave as *p*-type semiconductor.
- High water adsorption energy is found for Se_BiVO₄

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