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Enhanced driving force and charge separation efficiency in disordered  $\text{SnNb}_x\text{O}_y$ :

Boosting photocatalytic activity toward water reduction

Shushu Huang,<sup>a</sup> Junyu Lang,<sup>a</sup> Chunfang Du,<sup>a</sup> Fenggang Bian,<sup>b</sup> Yiguo Su<sup>\*a</sup> and Xiaojing Wang<sup>\*a</sup>

<sup>a</sup>*College of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot, Inner Mongolia 010021, P. R. China*

<sup>b</sup>*Shanghai Synchrotron Radiation Facility, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 200240, P.R. China.*

# **Abstract:**

In this work, the disordered  $\text{SnNb}_x\text{O}_y$  with controlled structural distortion was developed in order to uncover the underlying origination for highly enhanced photocatalytic activity of the disordered materials. Synchrotron radiation wide-angle X-ray scattering (SR-WAXS) and transmission electron microscopy (TEM) results indicated that the as-prepared catalysts show disordered features with controlled short range ordering limits. In combination with optical diffuse reflectance spectra, valence band X-ray photoelectron spectroscopy (VB-XPS) and density functional theory (DFT) prediction, the disordered structure engineering can induce continuous band gap broadening and downward valence band edge, predicting enhanced oxidation driving force. Moreover, transient absorption spectroscopy (TAS), electron spin resonance (EPR) spectra suggested that the highly enhanced photocatalytic activity mainly originates from defect-assisted charge separation, which implies that abundant defective centers may serve as trap centers for efficient charge separation and improve charge transfer rate to suppress the charge recombination process. Photocatalytic test demonstrated that the optimal photocatalytic activity toward  $\text{H}_2$  evolution of the disordered catalyst shows ~11.7 times improvement with respect to that of the crystalline counterpart.

**Keywords:** photocatalysis; niobate; nanostructures; density functional calculations; disordered

Corresponding author: E-mail: cesyg@imu.edu.cn; wang\_xiao\_jing@hotmail.com;

Fax: +86-471-4992981; Tel: +86-471-4344579.

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