## Efficient Photocatalytic Reduction of Dinitrogen to Ammonia on

## **Bismuth Monoxide Quantum Dots**

Songmei Sun<sup>1</sup>, Qi An<sup>2</sup>, Wenzhong Wang<sup>1\*</sup>, Ling Zhang<sup>1</sup>, Jianjun Liu<sup>1\*</sup>, William A.

Goddard III<sup>2</sup>

<sup>1</sup>State Key Laboratory of High Performance Ceramics and Superfine Microstructure,

Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 200050, P.

R. China

<sup>2</sup>Division of Chemistry and Chemical Engineering, California Institute of Technology,

Pasadena, California 91125, United States

\*Address correspondence to wzwang@mail.sic.ac.cn, jliu@mail.sic.ac.cn

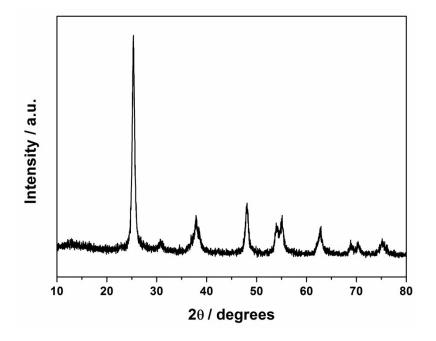


Figure S1 XRD pattern of the as-prepared 0.2%wt Fe-TiO<sub>2</sub> sample.

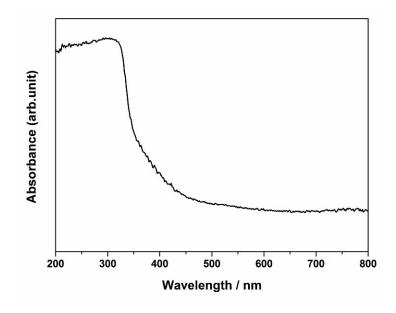


Figure S2. UV-vis diffuse reflection spectrum of the BiO particles.

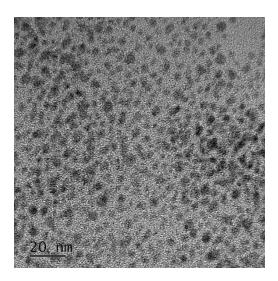


Figure S3 TEM image of the BiO quantum dots after cycles of photocatalytic reaction

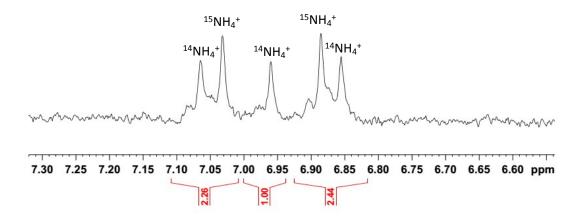


Figure S4  $^1H$  NMR spectrum of the obtained ammonia from photocatalytic  $N_2$  reduction using 50%  $^{15}N_2$  and 50%  $^{14}N_2$  as the purge gas.

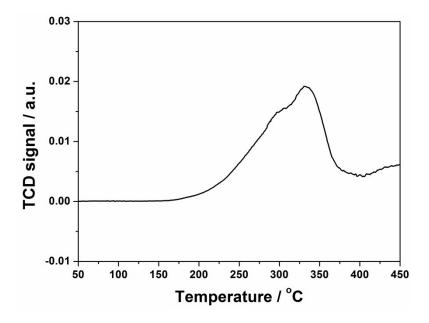


Figure S5 N<sub>2</sub>-TPD profiles of the as-prepared BiO catalyst.

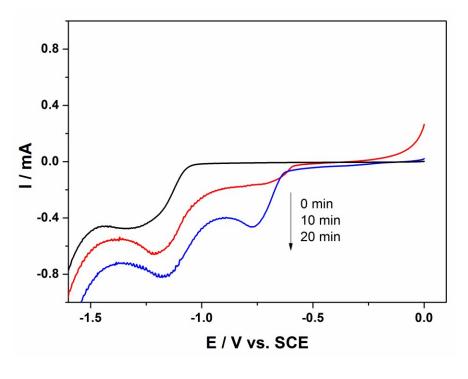


Figure S2

Figure S6 Changes of cathodic peaks for  $N_2$  reduction on BiO electrode along with the scan time in  $N_2$  saturated 0.5 M Na<sub>2</sub>SO<sub>4</sub> at pH 3.8. Scan rate: 100 mV/s.

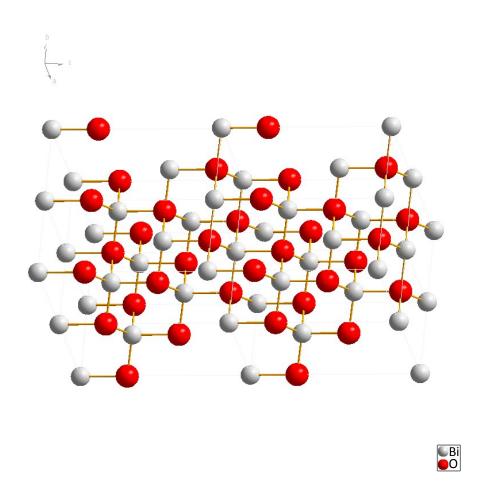


Figure S7 Schematic crystal structure of BiO which clearly shows the coordination environment of Bi and O atoms.

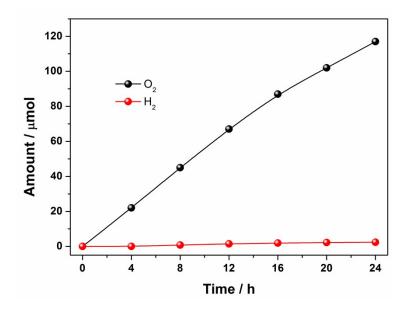


Figure S8 Hydrogen and oxygen evolution during the photocatalytic ammonia synthesis process in a closed reaction system.