Electronic supporting information

A Red Anatase TiO₂ Photocatalyst for Solar Energy Conversion

Gang Liu,^{1†} Li-Chang Yin,^{1†} Jianqiang Wang,² Ping Niu,¹ Chao Zhen,¹ Yingpeng Xie,¹ Hui-Ming Cheng¹*

¹ Shenyang National Laboratory for Materials Science, Institute of Metal Research,

Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China

² Shanghai Synchrotron Radiation Facility, Shanghai Institute of Applied Physics,

Chinese Academy of Sciences, 239 Zhangheng Road, Shanghai, 201800, China



Fig S1 XRD patterns of the white TiO_2 microspheres treated in gaseous ammonia atmosphere at different temperatures from 600 °C to 800 °C for 1 h.



Fig S2 XRD patterns of the (i) white and (ii) red TiO_2 microspheres. A: anatase; R: rutile.



Fig S3 UV-visible absorption spectra of the reference anatase TiO_2 without interstitial boron (i) before and (ii) after nitrogen doping.



Fig S4 Raman spectra of the (i) white and (ii) red TiO_2 microspheres.

Table 1 Comparing XPS binding energies of Ti 2p, O 1s, B 1s and N 1s in the white and red TiO_2 microspheres. The data was collected from the pristine surface.

Sample	Ti 2p (eV)	O 1s	N 1s	B 1s
	Percent (%)	Percent (%)	Percent (%)	Percent (%)
White TiO ₂	458.9	530.1		192.2
Red TiO ₂	458.3	529.5	397.6	191.6/190.1



Fig. S5 A $2 \times 2 \times 1$ supercell for anatase TiO₂.



Fig S6 The calculated band structures of anatase TiO_2 doped with $[BO_{4-x}N_x]$ (x = 4).



Fig S7 Plots of the transformed Kubelka–Munk function vs. the energy of light for the white and red TiO_2 microspheres.



Fig S8 GC signal spectra of H_2 detected in the gaseous product from the photoelectrochemical cell after different irradiation times.