Supplementary Information

Hydrogenated Black ZnO Nanoparticles with Enhanced Photocatalytic Performance

Ting Xia,^a Petra Wallenmeyer,^a Alicia Anderson,^a James Murowchick,^b Lei Liu,^{*,c} Xiaobo Chen^{*,a}

a Department of Chemistry, University of Missouri - Kansas City, Kansas City, Missouri 64110, USA;

b Department of Geosciences, University of Missouri - Kansas City, Kansas City, MO 64110, USA.

c State Key Laboratory of Luminescence and Applications, Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences, Changchun, 130033, People's Republic of China.

Experimental Section

Characterization. The XRD was performed using a Rigaku Miniflex XRD instrument with Cu K α as the X-ray sources (wavelength = 1.5418 Å). The Raman spectra were collected on an EZRaman-N benchtop Raman spectrometer with the excitation wavelength of 785 nm. The spectrum range was from 100 cm⁻¹ to 3100 cm⁻¹. The UV-visible reflectance spectra were collected with an Agilent Cary 60 UV-Vis spectrometer with a fiber optical reflectance unit. MgO power was used as the reference material. The ESR spectra were collected on a Benchtop Micro-ESRTM machine, at a microwave frequency of 9.70 GHz at room temperature without light irradiation. The ESR data were calibrated in relation to g = 2.0066 of 2,2,6,6-tetramethyl-4-hydroxylpiperidine-1-oxyl. The scanning time was 30 s per sweep, and the spectrum was averaged after 30 sweeps. Quartz ESR tubes with an inner diameter of 5.8 mm were used. The TEM study was performed on a FEI Tecnai F200 TEM with the electron accelerating voltage of 200 kV. A small amount of sample was dispersed in water, dropped onto a thin holey carbon film, and dried overnight before TEM measurement.

Photocatalytic testing. The photocatalytic activity was studied with the decomposition of methylene blue under simulated sunlight irradiation. The solar simulator had a 150 watt Xe lamp with an AM 1.5 air mass filter. 1.0 mg of catalyst was added into 3.0 ml methylene blue solution (optical density of 1.0). The UV-vis absorption spectrum of methylene blue was monitored at 664 nm over time after the photocatalytic reaction started.



Figure S1. XRD pattern of ZnO nanoparticles when calcined in air.

Using the FWHM values of the (100) and (002) peaks, we got 19.5 nm and 18.8 nm in the [100] and [001] directions, respectively, for the ZnO nanoparticles calcined in air. So the average crystalline grain size of was 19.1 nm.



Figure S2. (A) TEM and (B) HRTEM images of calcined ZnO nanoparticles.