Pure phase orthorhombic $MgTi_2O_5$ photocatalyst for H_2 production

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1. Quantum efficiency calculations

The determination of the apparent quantum efficiency for hydrogen generation was performed using the same closed circulating system under illumination of a 300 W Xe lamp with bandpass filter (313 nm) system. The light intensity was measured using a Si photodiode (oreal 91105V). The total light intensities were 36.69 $mW \cdot s^{-1}$ for 313 nm, 6.63 $mW \cdot s^{-1}$ for 365 nm. The irradiation area was around 7 cm^2. Apparent quantum efficiency (AQE) at different wavelengths was calculated by the following equation.

$$AQE = \frac{2 \times the\ number\ of\ evolved\ H_2 molecules}{the\ number\ of\ incident\ photons} \times 100\%$$

2. Solar to hydrogen (STH) conversion efficiency calculations from solar simulator measurements.

The solar energy conversion was evaluated by using AM 1.5 solar simulator as the light source with $MgTi_2O_5$ nanocrsytals as the catalyst (20 mg catalyst in 80 mL water and 20 ml methanol). After 1h of illumination, the total indident power over the 7 cm^2 irradiation area was 1.21 W, so that the total input energy in 1 hours was

$E_{Solar} = 4.36 \times 10^3$ J.

During the photocatalytic reaction, 94.72 μmol H_2 was detected by gas chromatography, which indicated that the energy generated by water splitting is E_F = 22.57 J.

$E_F = 94.72 \times 10^{-6} \times 6.02 \times 10^{23} \times 2.46 \times 1.609 \times 10^{-19}$; 2.46 eV is the free energy of water splitting.

The "solar-to-hydrogen" conversion efficiency of $MgTi_2O_5$ nanocrystals was determined to be:

$STH = E_F / E_{Solar} = 0.517\%$

Table S1. Control experiments to prepare pure phase $MgTi_2O_5$

Name	C_{Mg}(mol/L)	Molar Ratios		T(°C)	Production
		Mg	Ti		
PMT	0.0104	1	1	17	$MgTi_2O_5$
MMT-1	0.0104	1	2	17	Mixed phase
MMT-2	0.0104	2	1	17	Mixed phase
MMT-3	0.0278	1	1	17	Mixed phase
MMT-4	0.0278	1	2	25	Mixed phase

C_{Mg} is the concentration of Mg^{2+} ions in solution. Mixed phase contains $MgTiO_3$ and $MgTi_2O_5$.

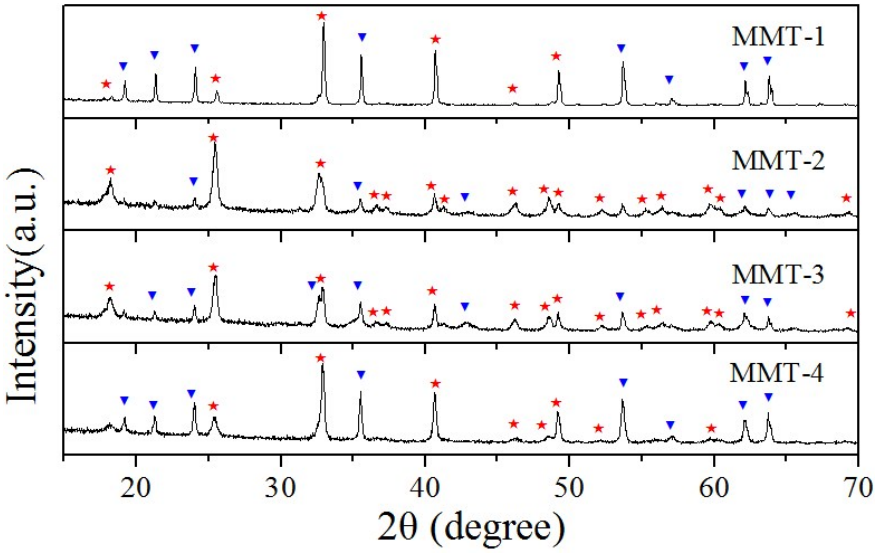

Figure S1. XRD patterns of mixed phase magnesium titanates (the red star is phase of $MgTi_2O_5$ and the blue triangle is phase of $MgTiO_3$).

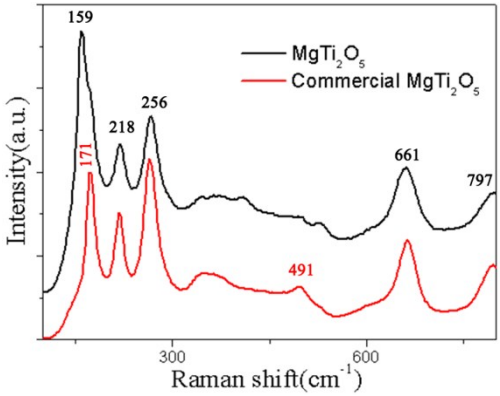

Figure S2. Raman spectra of $MgTi_2O_5$ nanocrystals and commercial $MgTi_2O_5$.

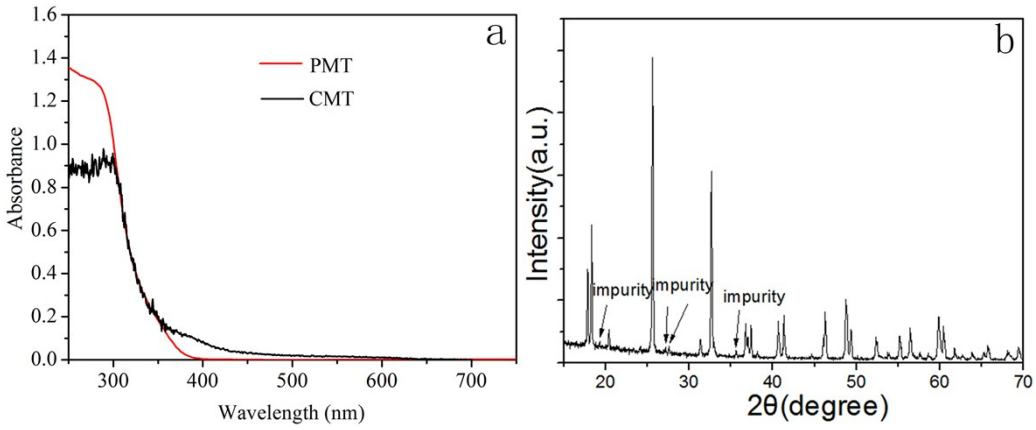

Figure S3. UV-vis absorption spectrum (a) of PMT and CMT, and XRD pattern of CMT (b).

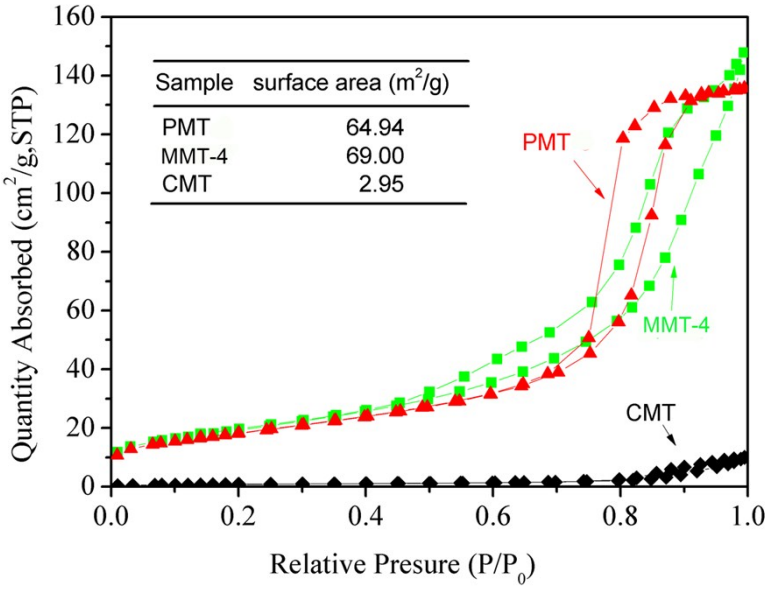

Figure S4. N_2 adsorption-desorption isotherm curves and pore size distribution (inset) of pure $MgTi_2O_5$ nanocrystals, mixed phase $MgTiO_3/MgTi_2O_5$ and commercial $MgTi_2O_5$.

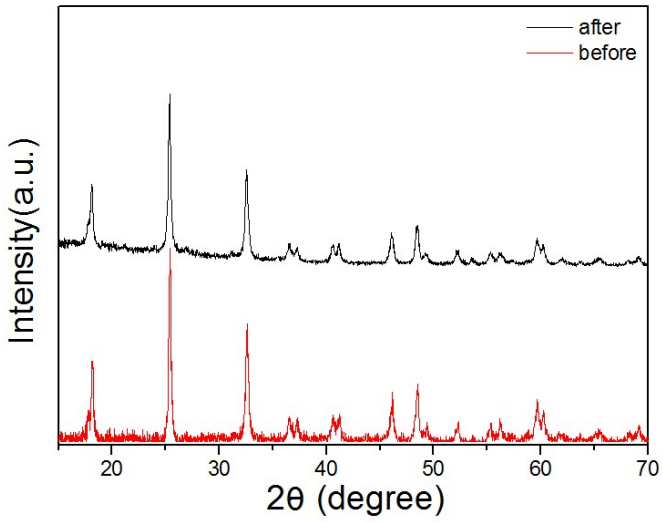

Figure S5. XRD patterns of PMT before and after five times recycles of H_2 production.