Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information (7 pages)

Aluminum Enhances Photochemical Charge Separation in Strontium Titanate Nanocrystal Photocatalysts for Overall Water Splitting

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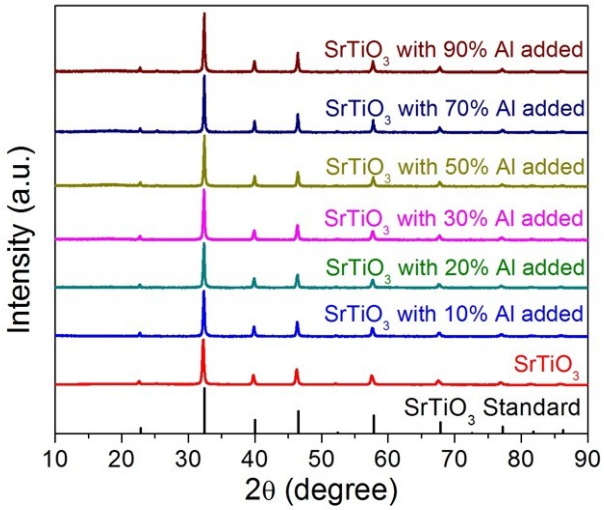

Figure S1 PXRD patterns of $SrTiO_3$ and Al:$SrTiO_3$ with different Al dopant amount obtained from hydrothermal synthesis with reference pattern for $SrTiO_3$ (JPDF #35-0734).

The unit cell change from nano-$SrTiO_3$ to 7.2 atom% nano-Al:$SrTiO_3$ is calculated based on Bragg's law. The ratio of 7.2 atom% nano-Al:$SrTiO_3$ unit cell to nano-$SrTiO_3$ unit cell is calculated based on Eq. (1) for all 7 peaks with 2θ from 20° to 70°. The average of 7 ratios shows that the unit cell of 7.2 atom% nano-Al:$SrTiO_3$ is 0.2% smaller than the unit cell of nano-$SrTiO_3$.

$$\frac{d(Al{:}SrTiO_3)}{d(SrTiO_3)} = \frac{sin(\frac{2\theta(SrTiO_3)}{2})}{sin(\frac{2\theta(Al{:}SrTiO_3)}{2})} \quad \text{Eq. (1)}$$

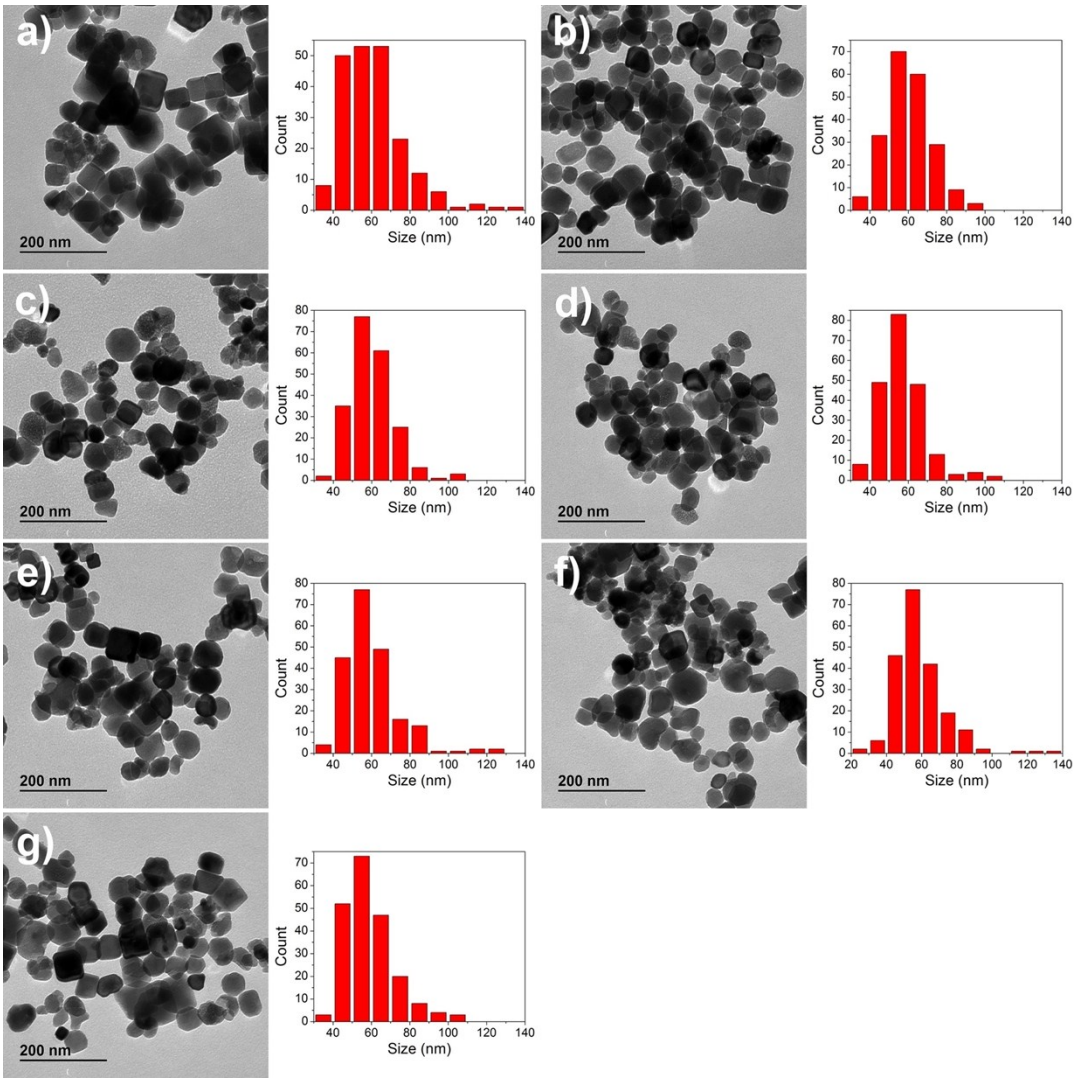

Figure S2 TEM images and size histograms of (a) nano-$SrTiO_3$ and nano-Al:$SrTiO_3$ with (b) 10%, (c) 20%, (d) 30%, (e) 50%, (f) 70% Al, (g) 90 atom% Al precursor added during the hydrothermal synthesis.

Table S1 XRF Results for Al:$SrTiO_3$.

	SrO wt%	TiO_2 wt%	Al_2O_3 wt%	2 [Al] / ([Sr]+[Ti]+[Al])
10% Al	55.6	43.5	0.905	3.2 %
20% Al	54.9	43.8	1.27	4.5 %
30% Al	54.6	44	1.36	4.8 %
50% Al	53.8	44.4	1.72	6.1 %
70% Al	52.6	45.3	2.04	7.2 %
90% Al	53.4	44.4	2.21	7.8 %
micro-Al:$SrTiO_3$	54.7	45.0	0.345	1.2%

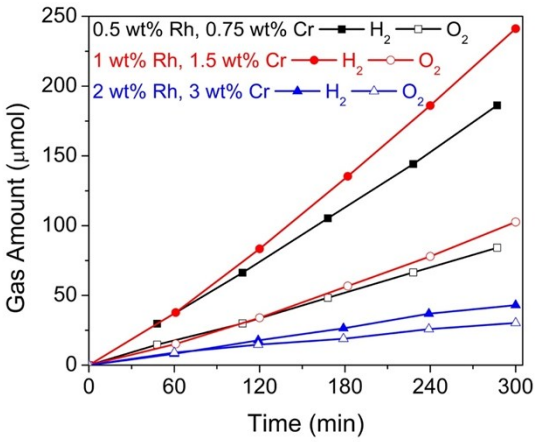

Figure S3 Irradiation results of 7.2% nano-Al:$SrTiO_3$ with variable amounts of $Rh_{2-y}Cr_yO_3$ co-catalyst in pure water under full spectrum of Xe lamp irradiation (240 mW/cm^2 by UV detector). Dots show H_2 amount while circles show O_2 amount.

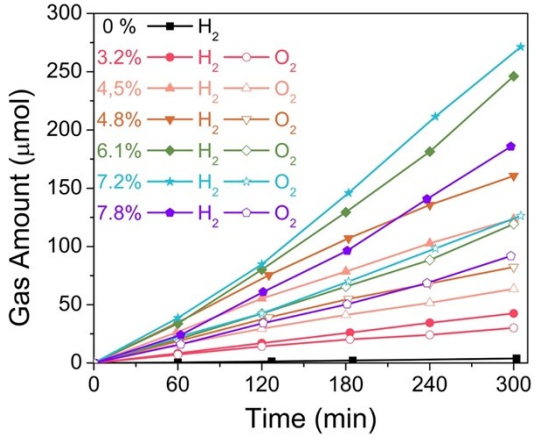

Figure S4 Irradiation results of 1wt% Rh, 1.5 wt% Cr, $Rh_{2-y}Cr_yO_3$ loaded nano-Al:$SrTiO_3$ with different amount of Al in pure water under full spectrum of Xe lamp irradiation (240 mW/cm^2 by UV detector). Dots show H_2 amount while circles show O_2 amounts.

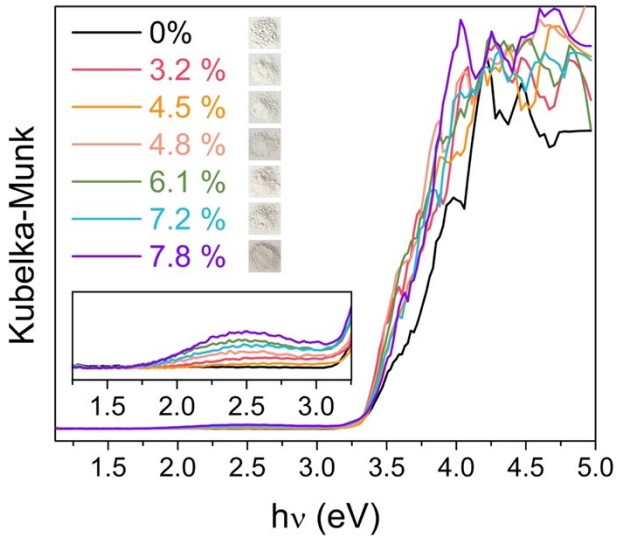

Figure S5 UV-Vis diffuse reflectance spectra of nano-Al:$SrTiO_3$ with variable Al^{3+} concentration with inset of their photos. The region from 1.25 eV to 3.25 eV is magnified to illustrate the weak absorption feature starting from 1.7 eV.

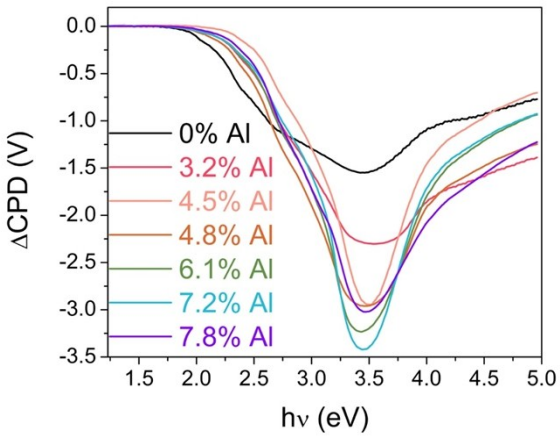

Figure S6 SPS spectra of nano-Al:$SrTiO_3$ with variable Al^{3+} concentration.

Calculation of the specific surface area for Al:$SrTiO_3$

The specific surface area (SSA) of the Al:$SrTiO_3$ catalyst was calculated assuming a cubic shape, with *a* as the length of the cube edge.

Eq. (2) $$SSA = \frac{6 \times a^2}{a^3} = \frac{6}{a}$$

Eq. (3) $$SSA\left(nano - Al{:}SrTiO_3\right) = \frac{6}{59.5 \times 10^{-9} m} = 1.01 \times 10^8 \frac{m^2}{m^3}$$

Eq. (4) $$SSA\left(flux - Al{:}SrTiO_3\right) = \frac{6}{343.4 \times 10^{-9} m} = 1.75 \times 10^7 \frac{m^2}{m^3}$$

To load same amount of co-catalyst per surface area on both nano-7.2% Al:$SrTiO_3$ and flux-Al:$SrTiO_3$,

Eq. (5) $$\frac{co - catalyst\left(nano - Al{:}SrTiO_3\right)}{SSA\left(nano - Al{:}SrTiO_3\right)} = \frac{co - catalyst\left(flux - Al{:}SrTiO_3\right)}{SSA\left(flux - Al{:}SrTiO_3\right)}$$

Because nano-7.2% Al:$SrTiO_3$ is loaded with 1.0 wt% Rh and 1.5 wt% Cr, flux Al:$SrTiO_3$ is loaded with 0.17 wt% Rh, 0.26 wt% Cr, $Rh_{2-y}Cr_yO_3$ to achieve same co-catalyst coverage per surface area.

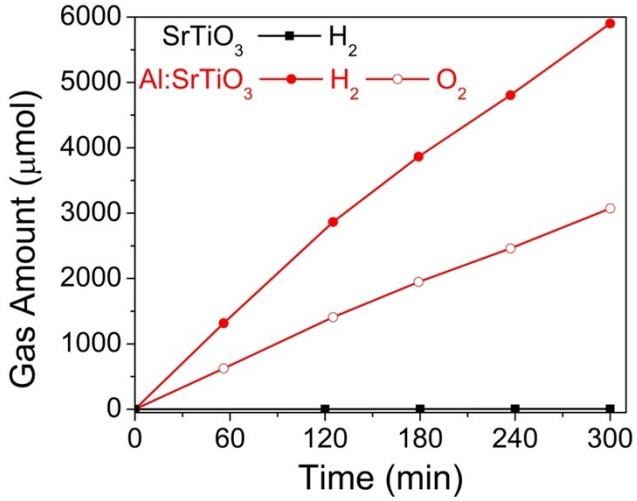

Figure S7 H_2/O_2 evolution from 0.1 wt% Rh, 0.1 wt% Cr, $Rh_{2-y}Cr_yO_3$ loaded ss-$SrTiO_3$ and micro-Al:$SrTiO_3$ in pure water under full spectrum Xe irradiation (320 mW/cm^2 by UV detector).

Table S2 Microprobe Results of micro-Al:$SrTiO_3$ microparticles.

	O At%	Al At%	Sr At%	Ti At%	2[Al]/ ([Sr]+[Ti]+[Al])*100%
micro-Al:$SrTiO_3$ Microprobe	60.5±0.7	0.4±0.5	18.2±2.1	20.9±1.3	2.1 %