

ESI

Enhanced photocatalytic activity of TiO₂ activated by doping Zr and modifying Pd

Shaolong Huang^a, Yanlong Yu^c, Yabin Yan^a, Jixiang Yuan^a, Shougen Yin^{*b} and Yaan Cao^{*a}

^aThe Key Laboratory of Weak-Light Nonlinear Photonics, Ministry of Education, TEDA Applied Physics Institute and School of Physics, Nankai University, Tianjin 300457, China

^bKey Laboratory of Display Materials and Photoelectric Devices (Ministry of Education); Institute of Material Physics, and Tianjin Key Laboratory for Photoelectric Materials and Devices, Tianjin University of Technology, Tianjin 300384, China

^cCollege of Chemistry, Department of Materials Chemistry, Nankai University, Tianjin 300457, China

*To whom correspondence should be addressed. E-mail: caoya@nankai.edu.cn, sgyin@tjut.edu.cn.

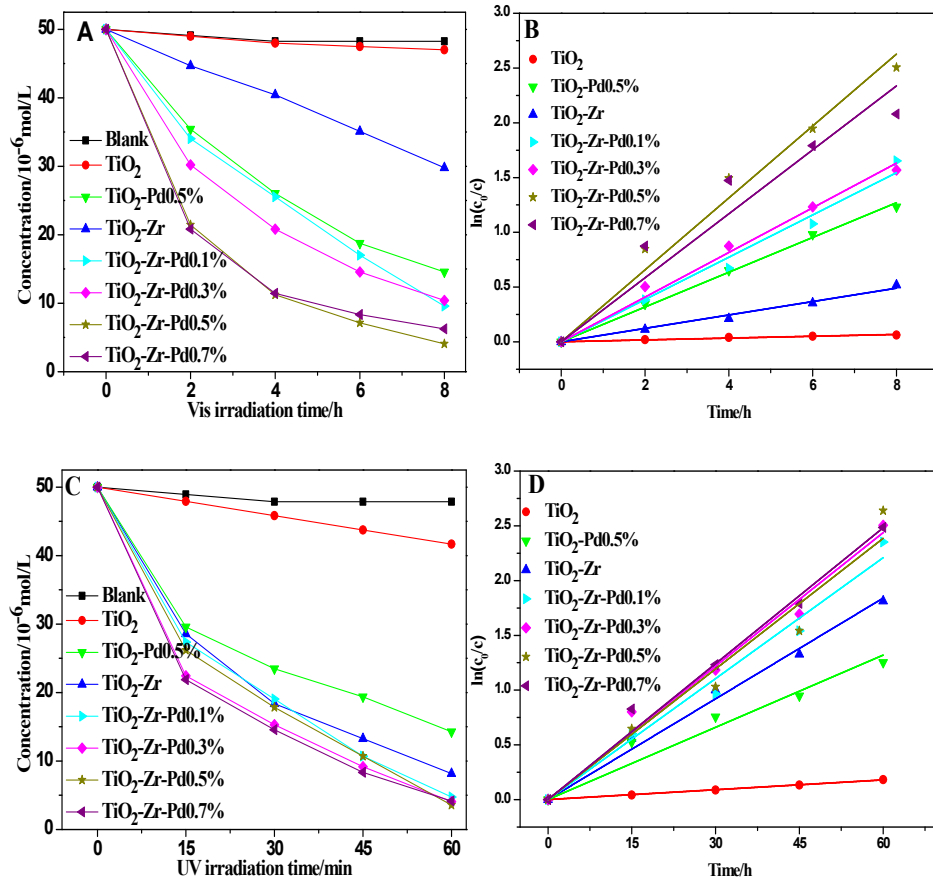


Figure S1. Photodegradation of 4-CP (A is under Vis irradiation and C is under UV irradiation) and relationship of $\ln(c_0/c)$ to reaction time (B is under Vis irradiation and D is under UV irradiation) for TiO₂, TiO₂-Pd0.5%, TiO₂-Zr and TiO₂-Zr-Pdx samples.

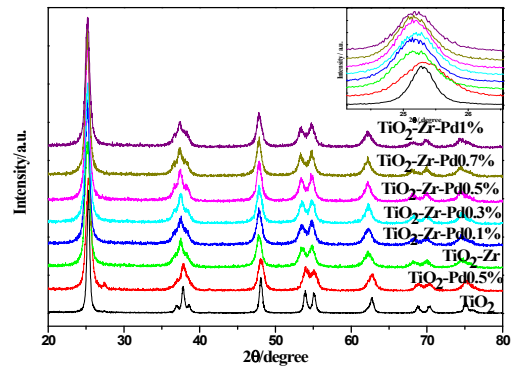


Figure S2. XRD patterns of TiO_2 , $\text{TiO}_2\text{-Pd}0.5\%$, $\text{TiO}_2\text{-Zr}$ and $\text{TiO}_2\text{-Zr-Pd}_x$ samples. The inset is the enlargement of the XRD peaks for the (1 0 1) plane.

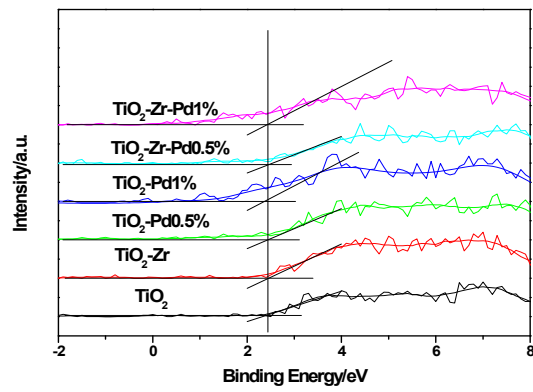


Figure S3. XPS valence band spectra for TiO_2 , $\text{TiO}_2\text{-Zr}$, $\text{TiO}_2\text{-Pd}0.5\%$, $\text{TiO}_2\text{-Pd}1\%$, $\text{TiO}_2\text{-Zr-Pd}0.5\%$ and $\text{TiO}_2\text{-Zr-Pd}1\%$ samples.

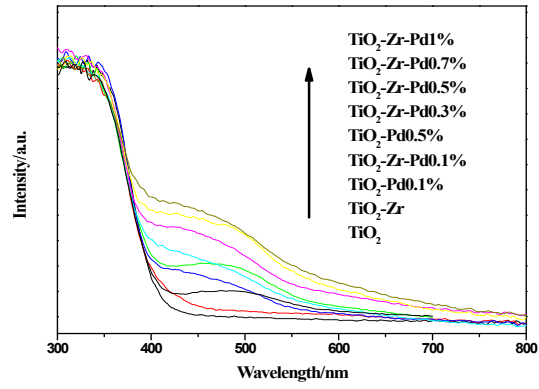


Figure S4. Diffuse reflectance UV-vis absorption spectra for TiO_2 , $\text{TiO}_2\text{-Pd}0.1\%$, $\text{TiO}_2\text{-Pd}0.5\%$, $\text{TiO}_2\text{-Zr}$ and $\text{TiO}_2\text{-Zr-Pdx}$ samples.

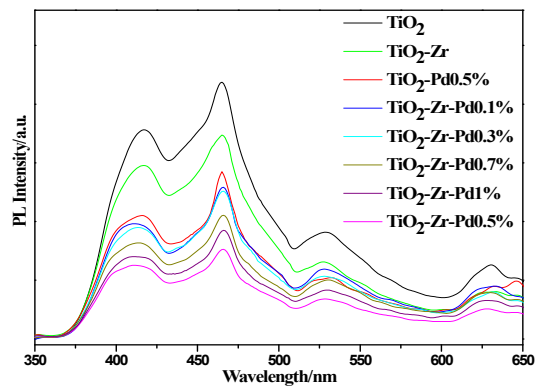


Figure S5. Photoluminescence spectra for TiO_2 , $\text{TiO}_2\text{-Pd}0.5\%$, $\text{TiO}_2\text{-Zr}$ and $\text{TiO}_2\text{-Zr-Pdx}$ samples.

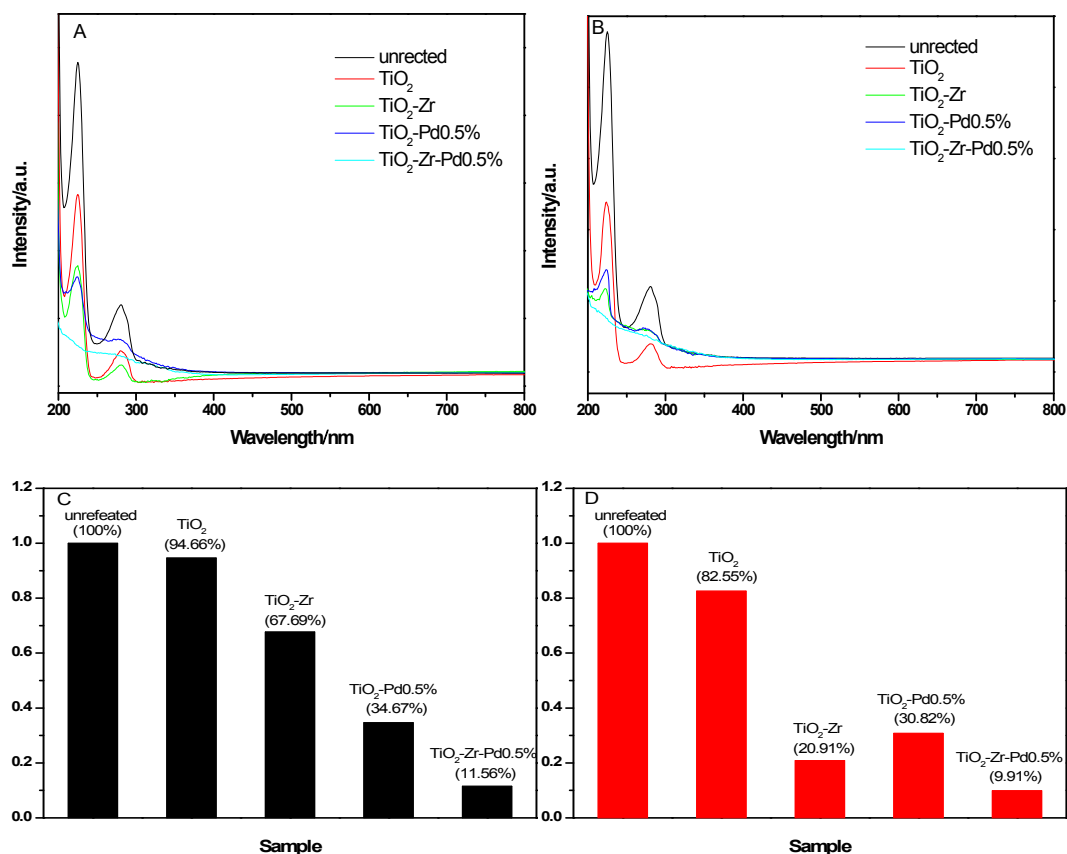


Figure S6. UV-Vis absorption spectra of the resultant reaction product under Vis irradiation (A) and UV irradiation (B) and the corresponding peak area of the absorption spectra (C is under Vis irradiation and D is UV irradiation) for TiO₂, TiO₂-Pd0.5%, TiO₂-Zr and TiO₂-Zr-Pdx samples.

The resultant reaction product can be measured by the UV-Vis absorption spectra after the irradiation. The absorption corresponding to the benzene ring (230 nm) decreases in the order of TiO₂ < TiO₂-Zr < TiO₂-Pd0.5% < TiO₂-Zr-Pd0.5% under Vis irradiation. Moreover, we use the peak areas of absorption spectra to represent the resultant amount of organic pollutants. It is found the fewest organic pollutants are detected for TiO₂-Zr-Pd0.5%, which is consistent with the discussion above (Figure 1).

Table S1. Lattice parameters, Cell volume, Crystal size and Specific surface area for TiO₂, TiO₂-Pd0.5%, TiO₂-Zr and TiO₂-Zr-Pdx samples.

Sample	Lattice parameters		Cell volume/Å ³	Crystal size/nm	Specific Surface Area
	a,b/Å	c/Å			
TiO ₂	3.783	9.501	136.0	13.0	63.8
TiO ₂ -Pd0.5%	3.781	9.499	135.8	12.6	75.4
TiO ₂ -Zr	3.802	9.540	137.9	11.3	85.1
TiO ₂ -Zr-Pd0.1%	3.802	9.554	138.1	11.8	83.3
TiO ₂ -Zr-Pd0.3%	3.803	9.542	138.0	11.1	87.0
TiO ₂ -Zr-Pd0.5%	3.804	9.551	138.2	12.3	81.0
TiO ₂ -Zr-Pd0.7%	3.803	9.562	138.3	12.0	83.1
TiO ₂ -Zr-Pd1%	3.801	9.573	138.3	11.5	84.4

Table S2. Eg for all the samples.

sample	TiO ₂	TiO ₂ -Zr	TiO ₂ -Pd0.1%	TiO ₂ Pd0.5%	TiO ₂ -Zr-Pd0.1%	TiO ₂ -Zr-Pd0.3%	TiO ₂ -Zr-Pd0.5%	TiO ₂ -Zr-Pd0.7%	TiO ₂ -Zr-Pd1%
Eg (eV)	3.10	3.08	3.08	3.10	3.08	3.08	3.08	3.06	3.04

Table S3. The lattice parameters and cell volume of TiO₂-Zr5%-Pd0.5%, TiO₂-Zr10%-Pd0.5% and TiO₂-Zr15%-Pd0.5%.

Sample	Lattice parameters		Cell volume /Å ³
	a,b/ Å	c/Å	
TiO ₂ -Zr5%-Pd0.5%	3.805	9.532	138.0
TiO ₂ -Zr10%-Pd0.5%	3.804	9.551	138.2
TiO ₂ -Zr15%-Pd0.5%	3.819	9.784	142.7

We have calculated the lattice parameters and cell volume of TiO₂-Zr5%-Pd0.5% and TiO₂-Zr15%-Pd0.5%. And it

is clear that the lattice parameters and cell volume increase with the Zr content.