Supporting information

Synthesis and Photocatalytic Activity of Cation-Doped Titanium Oxynitrides (Ti_{2.85-x} M_x O₄N, M = Zn, Co, Cu)

Qijing Gao ^a, Wenyan Shi ^{a, *}, Wenqian Chen ^{a, *}

a Key Laboratory of Organic Compound Pollution Control Engineering (MOF), School of Environmental and Chemical Engineering, Shanghai University, No. 99, Shangda Road, Shanghai 200444, China.

*Corresponding author. E-mail addresses: <u>wyshi1981@shu.edu.cn(W.</u>Y. Shi), wenqianchen@shu.edu.cn (W.

Q. Chen)



Figure S1. SEM images of oxides and oxynitrides doped with different cations: (a-d) Zn; (e-h) Co; (i-l) Cu.



Figure S2. EDS mapping spectrum of $Cs_{0.68}Ti_{1.83-x}Cu_xO_{4-y}N_y$ -600.



Figure S3. UV-visible diffuse reflection spectroscopy of (a) the oxides doped with different cations and synthesized oxynitrides at different temperatures (b) 500 $^{\circ}$ C; (c) 600 $^{\circ}$ C; (d) 700 $^{\circ}$ C.



Figure S4. Total density states (TDOS) and partial density states (PDOS) of (a) $Cs_{0.68}Ti_{1.83}O_4$ and (b) $Cs_{0.68}Ti_{1.83-x}Zn_xO_{4-y}N_y$ -600, (c) $Cs_{0.68}Ti_{1.83-x}Co_xO_{4-y}N_y$ -600, and (d) $Cs_{0.68}Ti_{1.83-x}Cu_xO_{4-y}N_y$ -600.



Figure S5. Nitrogen adsorption-desorption curves of (a) the oxides doped with different cations and (b) synthesized oxynitrides at 600 °C.



Figure S6. Transient photocurrent spectra of (a) $Cs_{0.68}Ti_{1.83-x}Zn_xO_{4-y}N_y$ -600 and (b) $Cs_{0.68}Ti_{1.83-x}Co_xO_{4-y}N_y$ -600



Figure S7. XPS spectrum of (a) Cu 2p (b) N 1s and (c) Cs 3d for $Cs_{0.68}Ti_{1.83}O_4$, $Cs_{0.68}Ti_{1.83-x}Cu_xO_4$, and $Cs_{0.68}Ti_{1.83-x}Cu_xO_{4-y}N_y$ -600 were etched with Ar ion clusters at 30 nm, and (d) ESR spectra for $Cs_{0.68}Ti_{1.83-x}Cu_xO_4$ and $Cs_{0.68}Ti_{1.83-x}Cu_xO_{4-y}N_y$ -600



Figure S8. Photocatalytic degradation efficiency plots of Zn- and Co-doped titanium oxides and titanium nitrogen oxides for the photocatalytic degradation of methylene blue.



Figure S9. XRD patterns of Cs_{0.68}Ti_{1.83-x}Cu_xO_{4-y}N_y-600 before and after photocatalytic reaction.

	Surface area $(m^2 g^{-1})$	Pore volume $(cm^{-3}g^{-1})$	Pore size (nm)
$Cs_{0.68}Ti_{1.83}O_4$	2.9837	0.0119	15.9533
$Cs_{0.68}Ti_{1.83-x}Zn_xO_4$	2.9236	0.0106	14.5027
$Cs_{0.68}Ti_{1.83-x}Co_xO_4$	11.2711	0.0277	9.8305
$Cs_{0.68}Ti_{1.83-x}Cu_xO_4$	12.1303	0.0671	22.1264
$Cs_{0.68}Ti_{1.83-x}Zn_xO_{4-y}N_y$ -600	7.2967	0.0544	29.8217
$Cs_{0.68}Ti_{1.83-x}Co_xO_{4-y}N_y$ -600	12.9577	0.0614	18.9540
$Cs_{0.68}Ti_{1.83-x}Cu_xO_{4-y}N_y$ -600	14.3266	0.0572	15.9703

 Table S1. The specific surface area and pore size of the oxides doped with different cations and synthesized oxynitrides at 600 °C.