

Supporting Information for

**Harmonious K-I-O Co-modification of g-C<sub>3</sub>N<sub>4</sub> for  
Improved Charge Separation and Photocatalysis**

Shifei Kang<sup>1#</sup>, Zhihao Zhang<sup>1#</sup>, Maofen He<sup>1</sup>, Zirou Fang<sup>1</sup>, Di Sun<sup>2</sup>, Lulu Zheng<sup>3</sup>,  
Xijiang Chang<sup>4\*</sup>, Lifeng Cui<sup>5\*</sup>

1. Department of Environmental Science and Engineering, University of Shanghai for Science and Technology, 200093, Shanghai, P.R. China

2. Department of Ultrasound in Medicine, Shanghai Jiao Tong University Affiliated Sixth People's Hospital & Shanghai Institute of Ultrasound in Medicine, Shanghai, 200233, P.R. China

3. Engineering Research Center of Optical Instrument and System, the Ministry of Education, Shanghai Key Laboratory of Modern Optical System, University of Shanghai for Science and Technology, Shanghai 200093, P.R. China

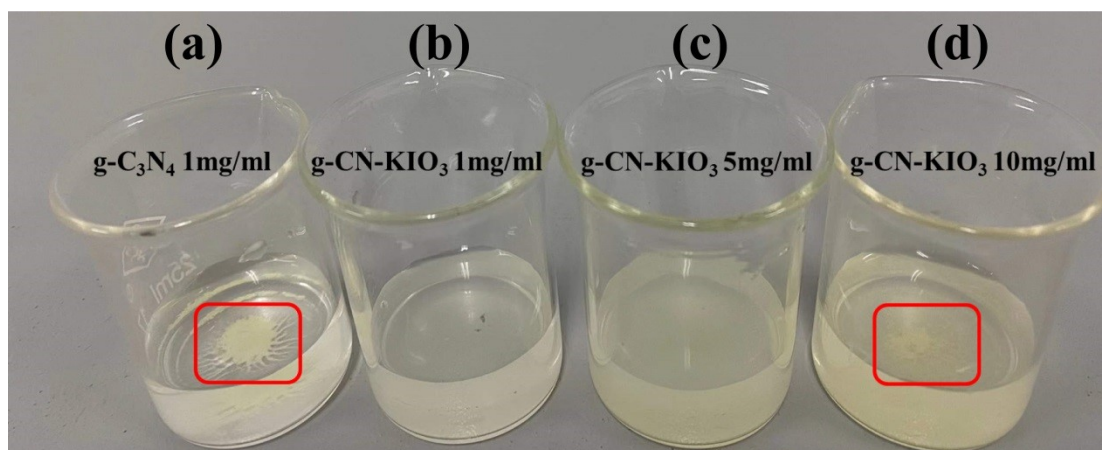
4. College of Science, Donghua University, Shanghai, 201620, P.R. China

5. College of Smart Energy, Shanghai Jiao Tong University, Shanghai, 200240, P.R. China.

# These authors contribute the same to this work.

\* Corresponding authors.

E-mail: changxj@dhu.edu.cn (Xijiang Chang), lifeng.cui@gmail.com (Lifeng Cui)



**Figure S1.** Photographs of (a)g-C<sub>3</sub>N<sub>4</sub> and (b-d)g-CN-KIO<sub>3</sub> water dispersions at different concentrations.

The specific experimental details are as follows: 10mg g-C<sub>3</sub>N<sub>4</sub> and g-CN-KIO<sub>3</sub> were weighed and added in 10ml water (1mg/ml), respectively. Stir the mixture for 10 minutes and let stand for 5 minutes. Undissolved g-C<sub>3</sub>N<sub>4</sub> powder can be obviously observed in Fig.S1a, while there is no residue of dissolved powder in medium g-CN-KIO<sub>3</sub> solution (Fig.S1 b). This phenomenon can be attributed to the excellent hydrophilic change caused by oxygen treatment. The maximum soluble concentration of g-CN-KIO<sub>3</sub> was further verified by put 50mg (Fig.S1 c) and 100mg (Fig.S1 d) g-CN-KIO<sub>3</sub> into 10ml water and repeat the above operations. It can be seen that when g-CN-KIO<sub>3</sub> is 100mg (10mg/ml), a small amount of g-CN-KIO<sub>3</sub> residue appeared. The solubility of g-CN-KIO<sub>3</sub> dispersion is 10 times better than that of the untreated g-C<sub>3</sub>N<sub>4</sub>.

**Table S1.** The atomic percentages of C, N, O, K and I in g-C<sub>3</sub>N<sub>4</sub> and g-CN-KIO<sub>3</sub>

	C(at.%)	N(at.%)	O(at.%)	K(at.%)	I(at.%)
g-C <sub>3</sub> N <sub>4</sub> (XPS)	48.06	50.17	1.77	-	-
g-CN-KIO <sub>3</sub> (EDS)	35.94	53.21	7.96	2.28	0.61
g-CN-KIO <sub>3</sub> (XPS)	46.93	48.39	2.50	1.98	0.20
g-CN-KIO <sub>3</sub> (ICP-MS)	-	-	-	1.71	0.45

Table S2. K/I/O doping optimization mechanism and its supporting evidences

	Optimization mechanism	Supporting evidence
K doping	1. The band structure adjustment	• The gap of 2.09 of g-CN-KiO <sub>3</sub> -2 is much smaller than that of 2.56 eV of g-C <sub>3</sub> N <sub>4</sub>
	2. Photoelectron chemical performance	• g-CN-KIO <sub>3</sub> has the highest photocurrent • The EIS of g-CN-KIO <sub>3</sub> is smaller than that of g-C <sub>3</sub> N <sub>4</sub>
	3. Accelerate the flow of charge	• The emission peak of g-CN-KiO <sub>3</sub> in PL spectrum is obviously weaker than that of g-C <sub>3</sub> N <sub>4</sub>
I doping	1. The enhanced electrical conductivity	• The EIS of g-CN-KIO <sub>3</sub> is smaller than that of g-C <sub>3</sub> N <sub>4</sub>
	2. Improve the surface electronic structure and charge carrier mobility	• g-CN-KIO <sub>3</sub> has the highest photocurrent • Compared to pure g-C <sub>3</sub> N <sub>4</sub> , g-CN-KIO <sub>3</sub> shows an enhanced EPR signal
Oxygen treatment	1. The band structure adjustment	• existence of mesopores
	2. Change the morphology	• TEM showed surface pores in g-CN-KiO <sub>3</sub>
	3. The increase of C-O species	• XPS spectra show that the concentration of O atom increases
	4. Enhanced hydrophilicity	• The solubility dispersion is almost 10 times that of the untreated g-C <sub>3</sub> N <sub>4</sub> .