Supporting Information

The activation of oxygen through oxygen vacancy in BiOCl/PPy to inhibit toxic intermediates and enhance the activity of photocatalytic nitric oxide removal

Ziyan Zhao^{a,b,#}, Yuehan Cao^{b,#}, Fan Dong^c, Fan Wu^b, Bangxin Li^b, Qian Zhang^b, Ying Zhou^{a,b*}

a. State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu 610500, China

b. The Center of New Energy Materials and Technology, School of Materials Science and Engineering, Southwest Petroleum University, Chengdu 610500, China

c. Chongqing Key Laboratory of Catalysis and New Environmental Materials, College of Environment and Resources, Chongqing Technology and Business University, Chongqing 40067, China

[#] Ziyan Zhao and Yuehan Cao contributed equally to this work.

*To whom correspondence should be addressed

Email: yzhou@swpu.edu.cn (Ying Zhou)

1. *k*-point convergence test



Fig. S1. The *k*-point convergence test.

2. Surface energy convergence test



Fig. S2. The surface energy convergence test.

3. The configurations of BiOCl (001) surface



Fig. S3. The main and vertical view of BiOCl structure (The yellow atom stands for the site of oxygen vacancy).

4. The XRD pattern of PPy



Fig. S4. XRD pattern of PPy.

5. Photo-induced currents



Fig. S5. Photo-induced currents of BiOCl and BiOCl/PPy under visible light.

6. Configurations of NO oxidation on BiOCl and Ov-BiOCl surface



Fig. S6. The structures corresponding to the reaction path on BiOCl (a-c) and Ov-BiOCl (d-f) surface. (Lengths in Å.)



7. Photocatalytic NO oxidation evaluation

Fig. S7 Long-time test of BiOCl/PPy (0.75%) composites under visible light (>420 nm)



Fig. S8 Recycle experiment of BiOCl/PPy (0.75%) composites under visible light (>420 nm).

8. The unit parameters of BiOCl crystals

Crystal	Lattice parameters	Lattice parameters
	in calculations	in experiments
		(PDF#06-0249)
BiOC1	<i>a</i> = <i>b</i> =3.890, <i>c</i> =7.370	<i>a</i> = <i>b</i> =3.891, <i>c</i> =7.369
	<i>α=β=γ=</i> 90	<i>α=β=γ=</i> 90

Table S1. The unit parameters of BiOCl crystal. (Lengths in Å, angles in °.)