Electronic Supplementary Material (ESI) for RSC Advances.


Research Highlights of "**Multifunctional property exploration: $Bi_4O_5I_2$ with highly visible light photocatalytic performance and large nonlinear optical effect**"

**Fig. S1** EDS patterns of BiOI (a) and $Bi_4O_5I_2$ (b) samples

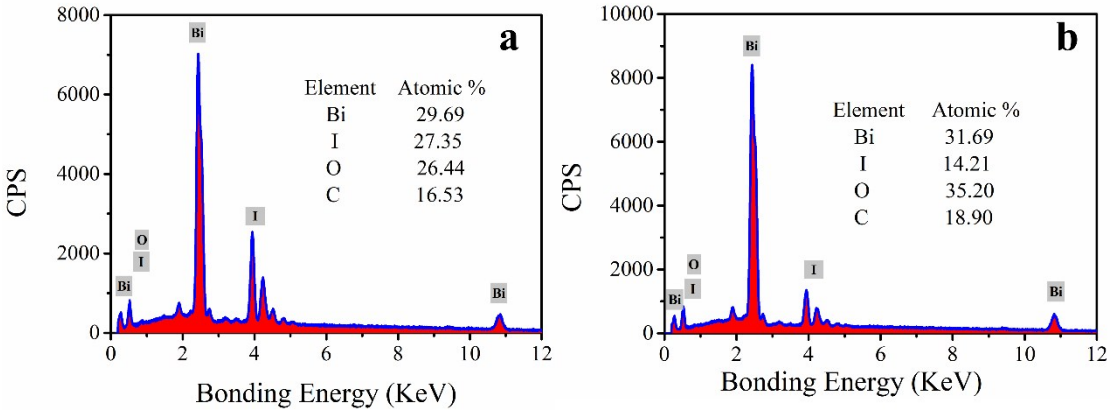

**Fig. S2** Photocatalytic activity of Blank (the initial concentration of 10 mg/L, catalyst is 50mg and without light), $Bi_4O_5I_2$, and P25 for degradation of MO under visible light irradiation (the initial concentration of 10 mg/L and amount of catalyst is 50mg) (a), effect of MO initial concentration on the photocatalytic performances of $Bi_4O_5I_2$ (b), photocatalytic degradation of MO, RhB, MB over BiOI and $Bi_4O_5I_2$ samples, respectively (c), photocatalytic activity of $Bi_4O_5I_2$ for degradation of norfloxacin under visible light irradiation (d)

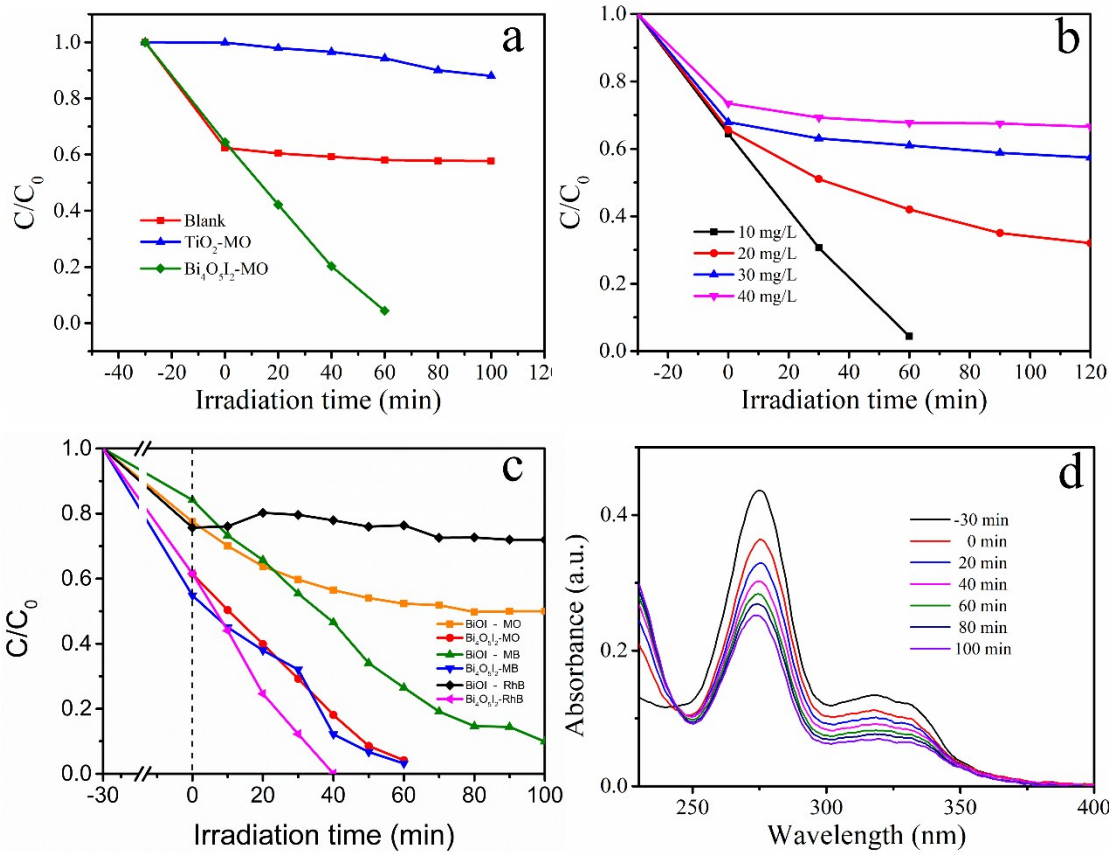

**Fig. S3** Free radicals trapping experiment of $Bi_4O_5I_2$ photocatalysts under visible light irradiation (a), Recycling property of $Bi_4O_5I_2$ photocatalyst (b), PL spectra of BiOI and $Bi_4O_5I_2$ (c), Mott-Schottky plots of the $Bi_4O_5I_2$ samples (d)

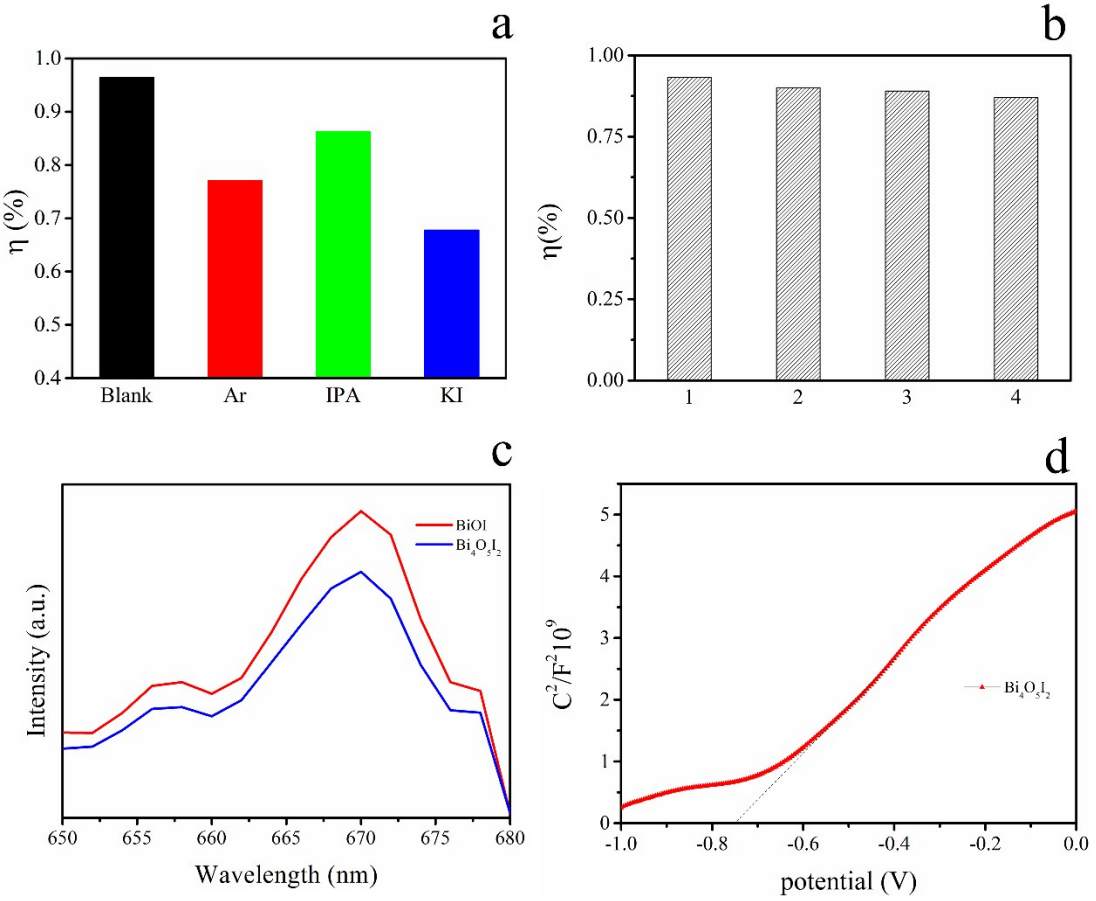


**Table ESI-1.** Pseudo-first-order kinetics parameter of MO

| | Pseudo-First-Order reaction | | |
|---|---|---|---|
| catalyst | $k_{app}$ ($min^{-1}$) | $R^2$ | Stansard error |
| BiOI | 0.0042 | 0.8636 | 0.0005 |
| $Bi_4O_5I_2$ | 0.0443 | 0.9237 | 0.0052 |

An internal polar electric field is constructed along the *ab* plane in the crystal structure of $Bi_4O_5I_2$ and the alignment of $BiO_4I_4$, $BiO_5I_3$, $BiO_6I$, $BiO_3I_4$ and $BiO_3I_5$ polyhedron in an individual polyhedra.

The bond-valence-sum Vi for each atom i is defined as

$$V_i = \sum_{\mathrm{j}} \mathrm{S_{ij}} = \sum \exp[\frac{R_0 - R_{ij}}{B}]$$

where B is a constant with value 0.37. R0 and Rij represent the reference and actual lengths of the bond i-j that the atom i makes with the surrounding atoms j, respectively, and Sij is the corresponding bond valence. R represents the difference between the "centroids" of the positive ($r^+$) and negative charges ($r^-$).

$$R = r^+ - r^-$$

For a given Bii-Oj bond with the actual bond length Rij, the nuclear charges of Bi and O are 83 and 8, respectively

$$(83 - V_i) \times r^- = (8 + S_{ij}) \times (R_{ij} - r^-)$$

Then, in units of Debye, in which R is measured by Å and the charge by statcoulomb, the net bond dipole moment $\mu_{ij}$ of the Bii-Oj bond is then calculated using the expression

$$\mu_{ij} = n_{ij} e R$$

$$n_{ij} = (83 - V_i) + (8 + S_{ij})$$

where $n_{ij}$ is the number of electrons forming the Bii-Oj, and e the electron charge (i.e., $4.8\times 10^{-10}$statcoulombs in cgs unit)

**Table ESI-2.** Dipole moments of $BiO_4I_4$, $BiO_5I_3$, $BiO_6I$, $Bi(1)O_3I_4$ , $BiO_3I_5$ polyhedra in $Bi_4O_5I_2$ crystal

| Polyhedral Unit | $Bi(1)O_4I_4$ | $Bi(3)O_4I_4$ | $Bi(1)O_5I_3$ | $Bi(3)O_5I_3$ | $Bi(1)O_6I$ | $Bi(3)O_6I$ | $Bi(1)O_3I_4$ | $Bi(1)O_3I_5$ | total |
|---|---|---|---|---|---|---|---|---|---|
| Polyhedral Moment (esu·cm/Å^3) | 0.149 | 0.141 | 0.117 | 0.118 | 0.069 | 0.065 | 0.163 | 0.12 | |
| X | -18.75 | -17.4 | -22.08 | -13.37 | 9.79 | -5.09 | -14.29 | -1.74 | |
| Y | 0.76 | 0.82 | 3.3 | -7.37 | -6.68 | 5.51 | 2.28 | -3.32 | |
| Z | 26.71 | 25.64 | 12.79 | -8.45 | 11.42 | 25.99 | -33.42 | 27.62 | |
| Polyhedral Unit | $Bi(2)O_4I_4$ | $Bi(4)O_4I_4$ | $Bi(2)O_5I_3$ | $Bi(4)O_5I_3$ | $Bi(2)O_6I$ | $Bi(4)O_6I$ | $Bi(2)O_3I_4$ | $Bi(2)O_3I_5$ | |
| Polyhedral Moment (esu·cm/Å^3) | 0.149 | 0.141 | 0.117 | 0.118 | 0.069 | 0.065 | 0.163 | 0.12 | |
| X | 18.75 | 17.4 | 22.08 | 13.37 | -9.79 | 5.09 | 14.29 | 1.74 | 0 |
| Y | 0.76 | 0.82 | 3.3 | -7.37 | -6.68 | 5.51 | 2.28 | -3.32 | -9.4 |
| Z | -26.71 | -25.64 | -12.79 | 8.45 | -11.42 | -25.99 | -33.42 | -27.62 | 0 |