Supporting Information

A Novel Nanoreactor Framework of Iodine-Incorporated BiOCl Core-Shell Structure: Enhanced Light-Harvesting System for Photocatalysis

Kun Zhang, Dieqing Zhang, Jie Liu, Kuaixia Ren, Hui Luo, Yingjie Peng, Guisheng Li and Xibin Yu*

Shanghai Key Lab of Rare Earth Functional Materials, Department of Chemistry, Shanghai Normal University, Shanghai, 200234, China.

xibinyu@shnu.edu.cn

Table S1. Synthetic conditions for iodine-incorporated BiOCl hollow, core-shell and solid microspheres.

Structure	V (H_2O) (ml)	V ($BiCl_3$) (ml)	PVP (g)	citric acid monohydrate (g)	C (NaI) (mmol)	T (℃)	Time (h)
Hollow	196	4	0.020	0.380	0.910	80	3
Core-shell	196	4	0.020	0.380	1.350	80	3
Solid	196	4	0.020	0.380	2.720	80	3

Table S2. The domain crystal size of BiOCl hollow and I-BiOCl core-shell product (the formation process of products) obtained by Williamson-Hall Method (the volume-weighted size) through the Jade 6.0 software from the width of the peaks (2θ=25.86).

Structure	Crystalline size (nm) calculate by Williamson-Hall Method			
	30s	1min	4min	3hours
BiOCl Hollow	54±2	54±4	93±3	100±4
I-BiOCl Core-shell	51±2	60±2	84±2	＞100

Table S3. The structure, surface area, $n_{(Cl^-)}/n_{(I^-)}$, band gap and the photocatalytic performance of the iodine-incorporated BiOCl products.

Structure	surface area/ (m^2/g)	$n_{(Cl^-)}/n_{(I^-)}$	band gap /eV	C/C$_0$ visible light irradiation 10 min	30 min	50 min	70 min	90 min	solar light irradiation 10 min	30 min	50 min
Hollow	75.6	0.052	2.43	0.589	0.147	0.059	0.037	0.02	0.151	0	0
Core-shell	51.5	0.065	2.28	0.37	0.086	0.025	0.013	0.004	0.092	0	0
Solid	8.2	0.163	2.04	0.923	0.665	0.435	0.306	0.206	0.796	0.358	0.157

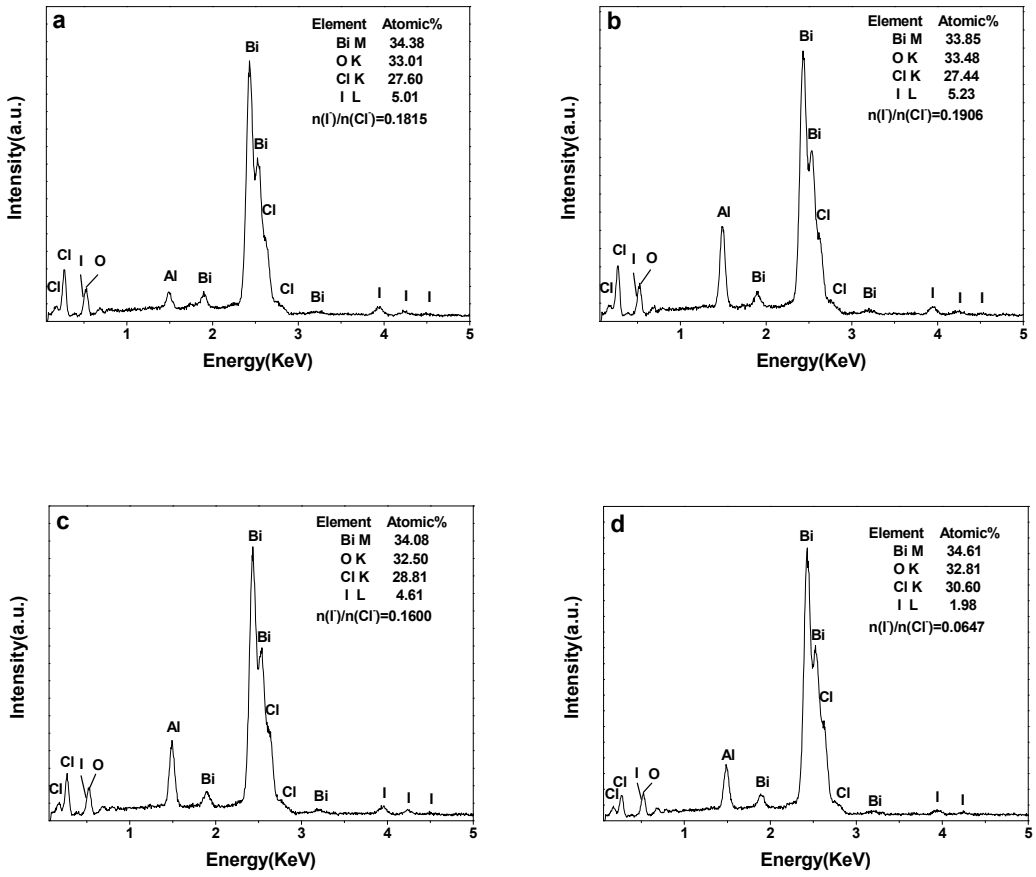


Fig. S1 EDS analysis of iodine-containing BiOCl core-shell microsphere produced in 1.350 mmol NaI solution at 80 ℃ for different times: (a) 30 sec, (b) 1 min, (c) 4 min, and (d) 3 hours.

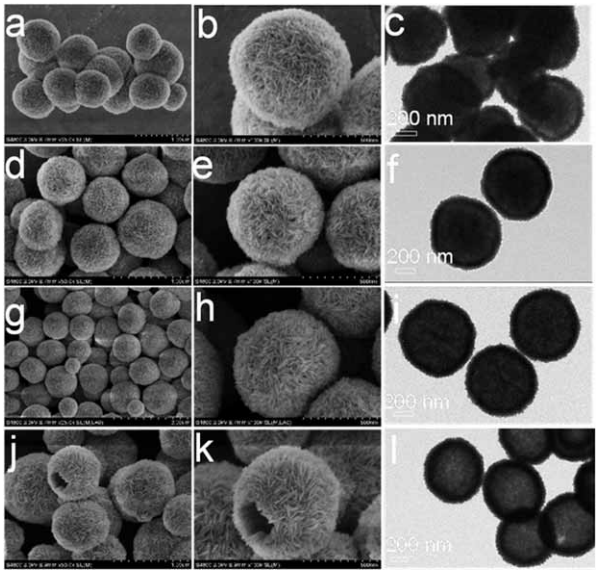


Fig. S2 FESEM and TEM images of pure BiOCl products without iodine-incorporation harvested at different intervals of reaction times, (a-c) 30 sec, (d-f) 1 min, (g-i) 4min, (j-l) 3hours.

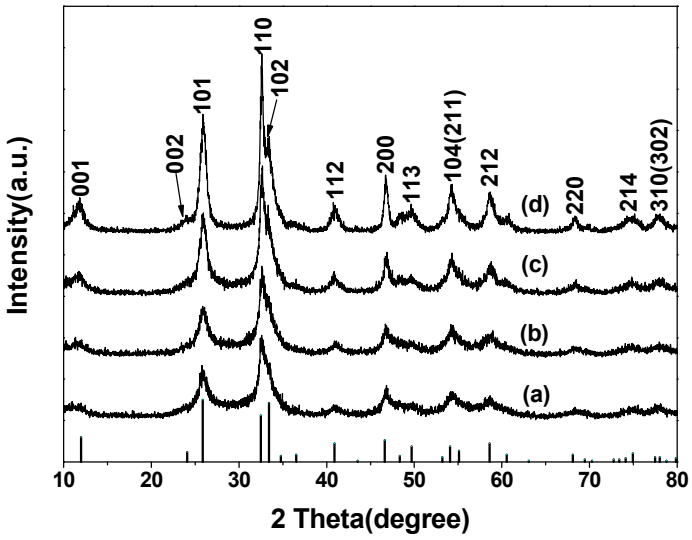


Fig. S3 XRD patterns of pure BiOCl products without iodine-incorporation harvested at different intervals of reaction times: (a)30s, (b)1min, (c)4min and (d)3hours (Inset the standard card: JCPDS 06-0249).

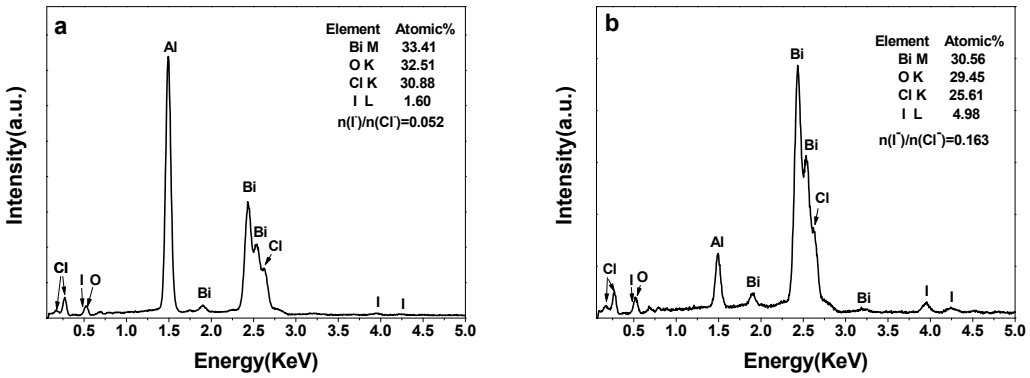


Fig. S4 EDS analysis on the atomic percentages of the iodine-incorporated (a) hollow and (b) solid BiOCl samples.

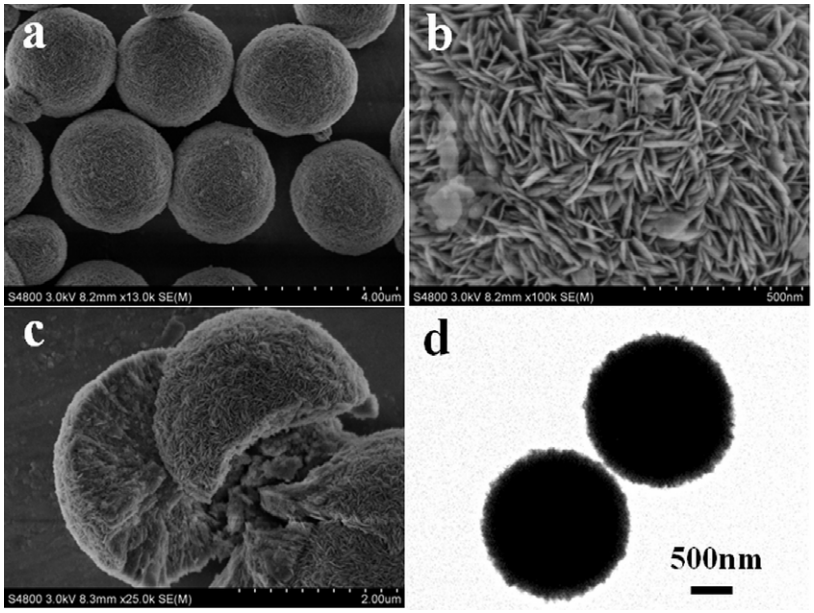


Fig. S5 (a-c) FESEM images of iodine-incorporation BiOCl (I-BiOCl) powders obtained without using PVP, (d) TEM images of iodine-incorporation BiOCl (I-BiOCl) powders.

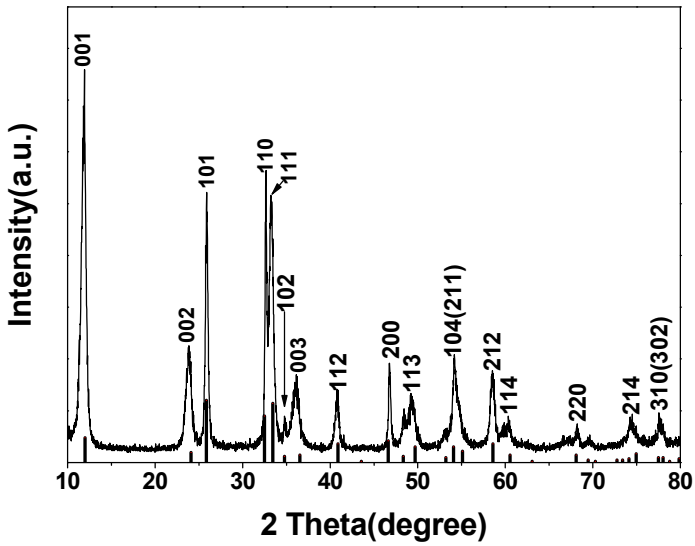


Fig. S6 XRD of iodine-incorporation BiOCl (I-BiOCl) powders obtained without using PVP. (Inset the standard card: JCPDS 06-0249)

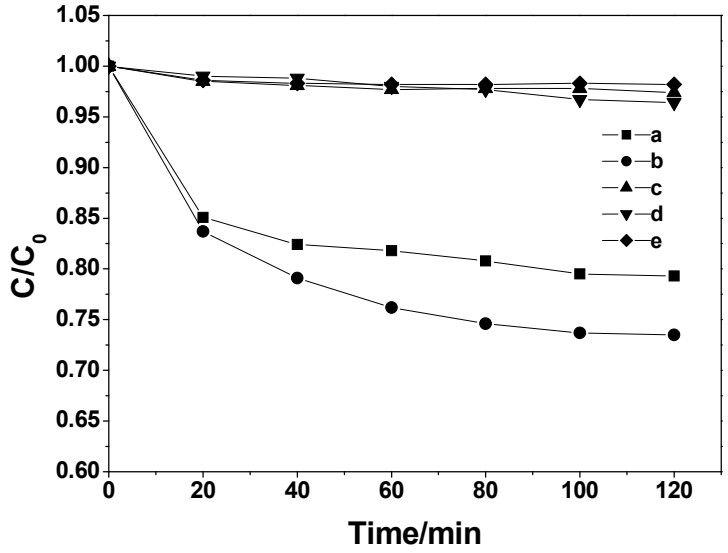


Fig. S7 Comparison of the adsorption-desorption equilibrium of iodine-incorporated BiOCl (I-BiOCl) with (a) hollow, (b) core-shell, (c) solid structure, (d) $TiO_{2-x-y}N_xF_y$(SC)-3 with (e) Bi_2WO_6.

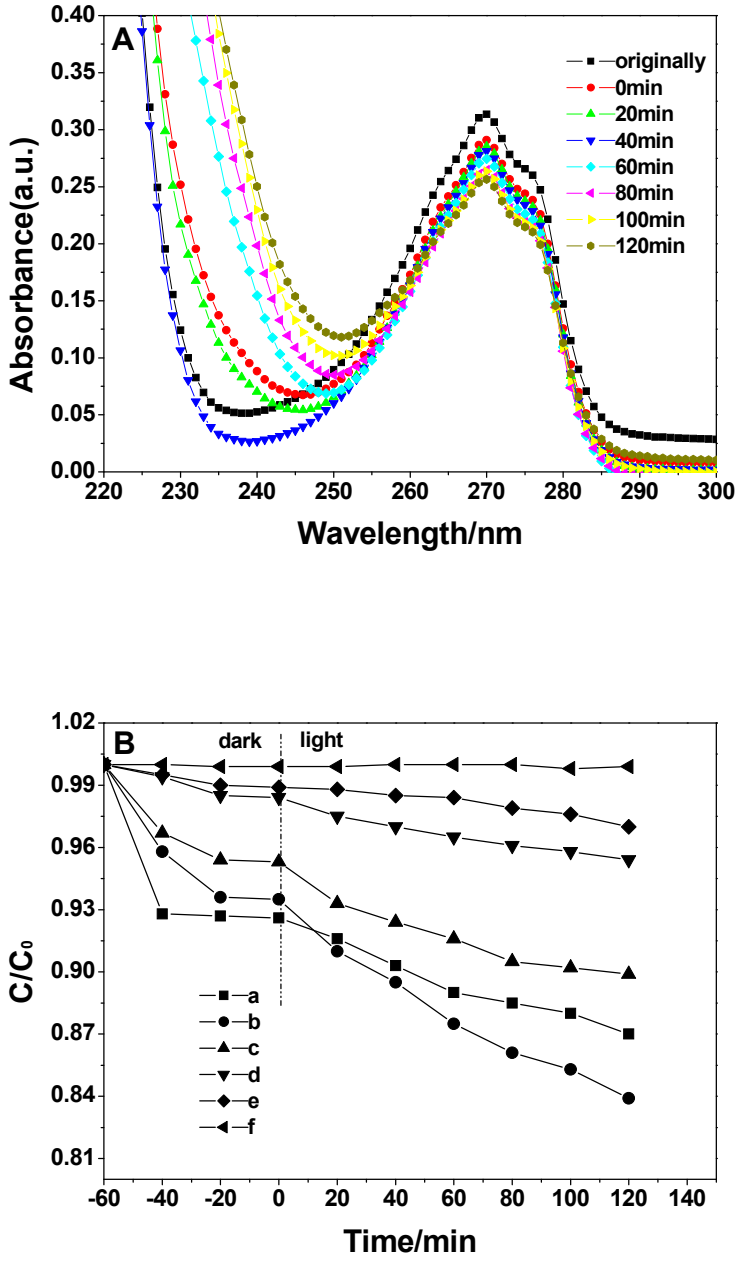


Fig. S8 (A) UV–vis absorption spectra of phenol over the 3D I-BiOCl core-shell microspheres during the photocatalytic process. (B)Comparison of visible-light photocatalytic activities of iodine-incorporated BiOCl (I-BiOCl) with (a) hollow, (b) shell-core, (c) solid structure, (d)$TiO_{2-x-y}N_xF_y$(SC)-3, (e) Bi_2WO_6 and (f) no catalyst on the degradation of 20 $mg \cdot L^{-1}$ phenol under visible-light irradiation (λ>420 nm). (75 W halogen-tungsten lamp as light source)

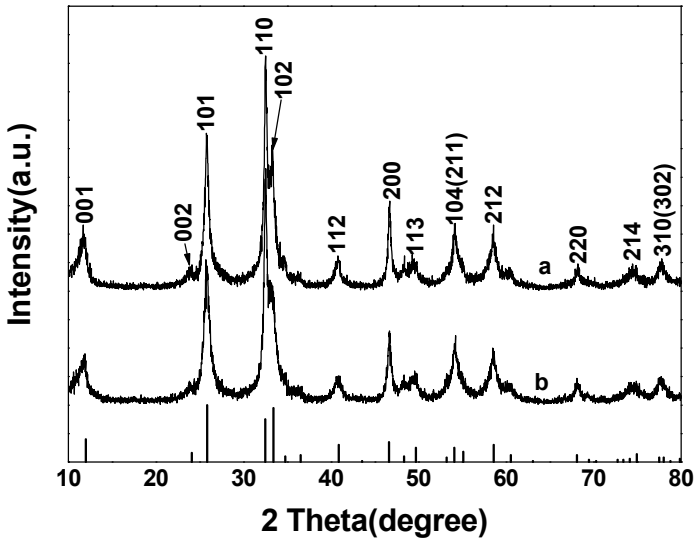


Fig. S9 XRD pattern of the iodine-incorporated core-shell BiOCl sample (a) before and (b) after the photocatalytic reaction. (Inset the standard card: JCPDS 06-0249)

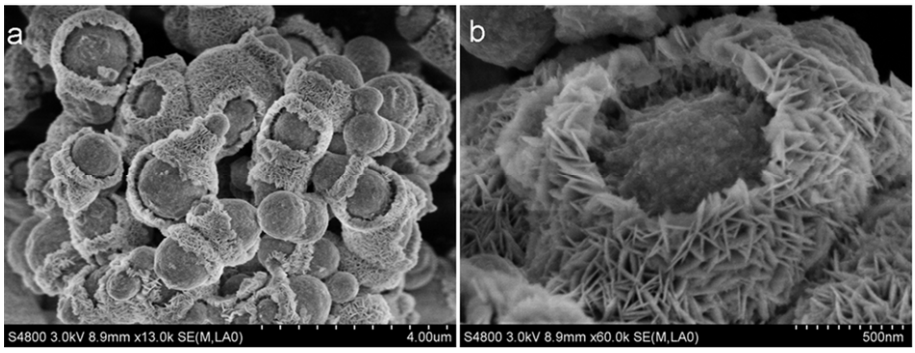
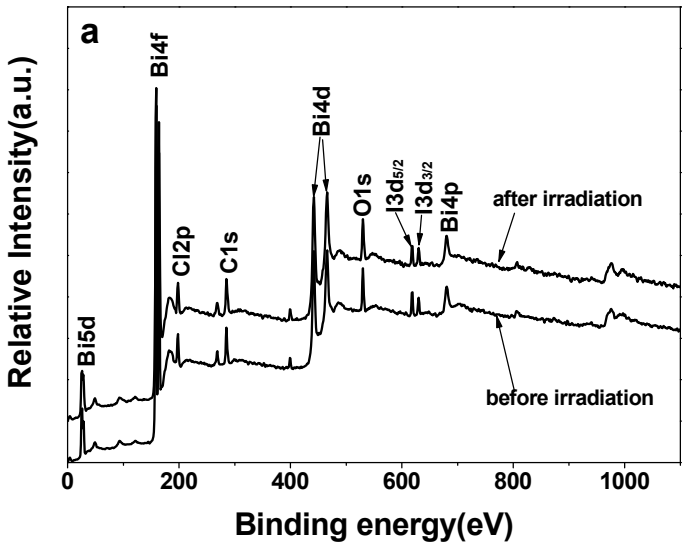
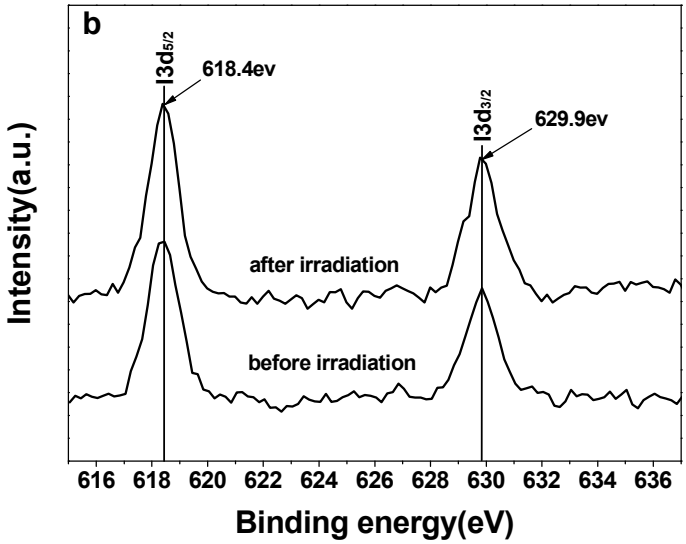


Fig. S10 FESEM images of the iodine-incorporated BiOCl core-shell sample after the photocatalytic reaction.


a
Bi4f
Bi4d
O1s
I3d5/2
I3d3/2
Bi4p
Cl2p
C1s
Bi5d
after irradiation
before irradiation
Relative Intensity(a.u.)
0
200
400
600
800
1000
Binding energy(eV)


b
I3d5/2
618.4ev
I3d3/2
629.9ev
after irradiation
before irradiation
Intensity(a.u.)
616
618
620
622
624
626
628
630
632
634
636
Binding energy(eV)

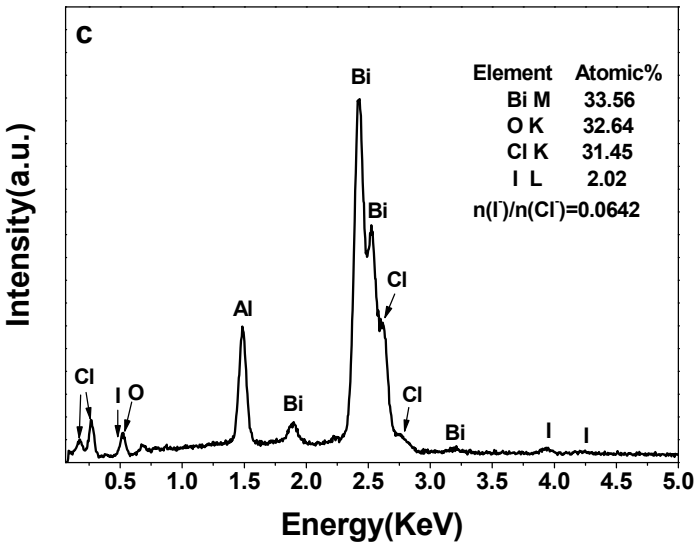


Fig. S11 (a) XPS survey spectrum of iodine-incorporated BiOCl core-shell sample before and after irradiation, (b) high-resolution XPS spectra of the I3d region taken on the iodine-incorporated BiOCl core-shell sample before and after irradiation, (c) EDS analysis on the atomic percentages of the iodine-incorporated core-shell sample after irradiation.

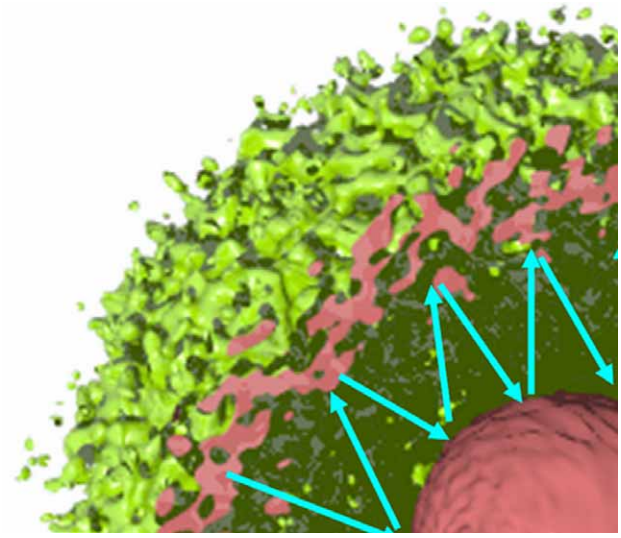


Fig. S12 Proposed model of light transfer paths, reflection, and scattering processes within the hierarchically core-shell structure.

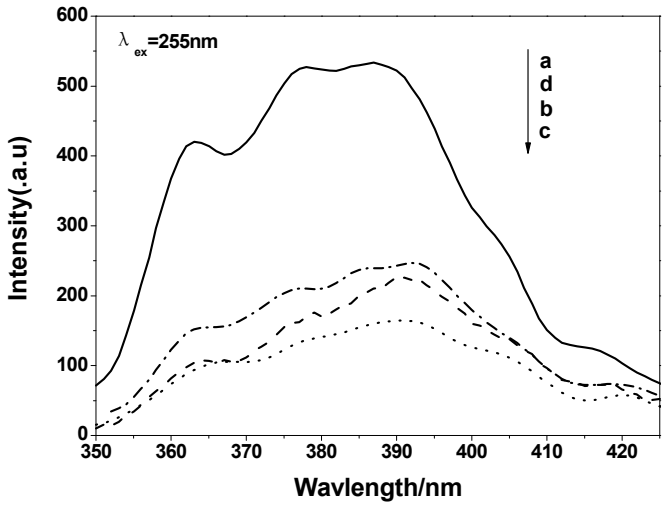


Fig. S13 PL spectra of BiOCl hollow microspheres (a) and iodine-containing BiOCl with (b) hollow, (c) shell-core, and (d) solid structure.