

Electronic Supplementary Information (ESI)

Supramolecular inclusion complexes of β -cyclodextrin with bathochromic-shifted photochromism and photomodulable fluorescence enable multiple applications

Dong-Xue Xia,^a Li-Wen Fan,^a Ming-Fu Ye,^{a, b} Wen-Qi Sun,^{a*} Rui-Lian Lin,^a and Jing-Xin Liu^{a*}

a. College of Chemistry and Chemical Engineering, Anhui University of Technology, Maanshan 243002, China. E-mail: jxliu411@ahut.edu.cn (J.X. Liu); wenqisun@sohu.com (W.Q. Sun)

b. AnHui Province Key Laboratory of Chemistry for Inorganic/Organic Hybrid Functionalized Materials, Anhui University, Hefei 230601, China.

Table of Contents

Figure S1-S2. ¹ H NMR and ¹³ C NMR spectra for viologens 3·Cl ₂ and 1·Cl ₂	S2,S3
Figure S3. 2D gCOSY NMR of three viologens.....	S4
Figure S4. ¹ H NMR spectra of 1 ²⁺ binding with β -CD.....	S5
Figure S5. ¹ H NMR spectra of 2 ²⁺ binding with β -CD.....	S6
Figure S6. Photographs of three viologens before and after irradiation.....	S7
Figure S7. Photographs of surface and internal colors of the inclusion complexes after irradiation.....	S8
Figures S8-S10. Electron distributions on HOMO and LUMO of the inclusion complexes.....	S9-S11
Figures S11-S13. FI-IR spectra of the inclusion complexes before and after irradiation.....	S12-S14
Figure S14. Photomodulable fluorescence of the 1 ²⁺ @ β -CD.....	S15
Figure S15. Photomodulable fluorescence of the 2 ²⁺ @ β -CD ₂	S16
Table S1 and S2. The customized codebook.....	S17

Figure S1. ^1H NMR and ^{13}C NMR spectra for viologen $\mathbf{3}\cdot\text{Cl}_2$.

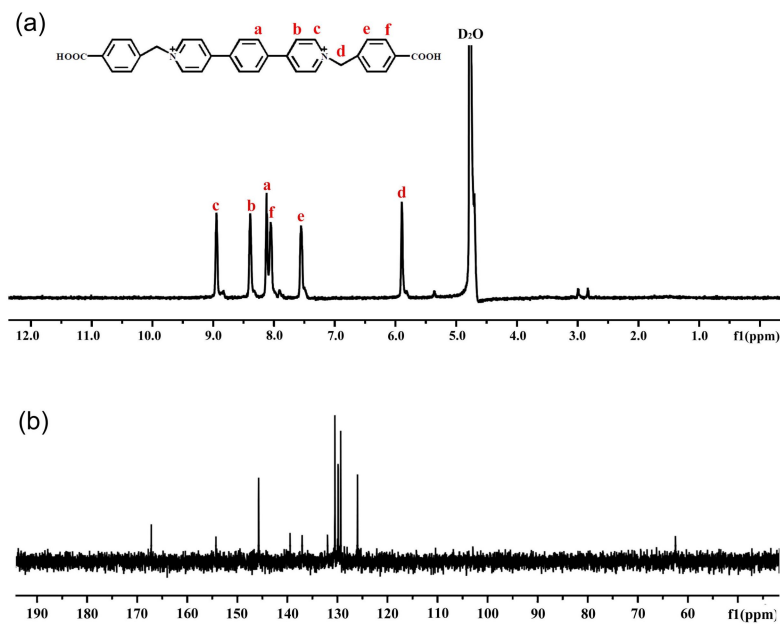


Figure S2. ^1H NMR and ^{13}C NMR spectra for viologen $1\cdot\text{Cl}_2$.

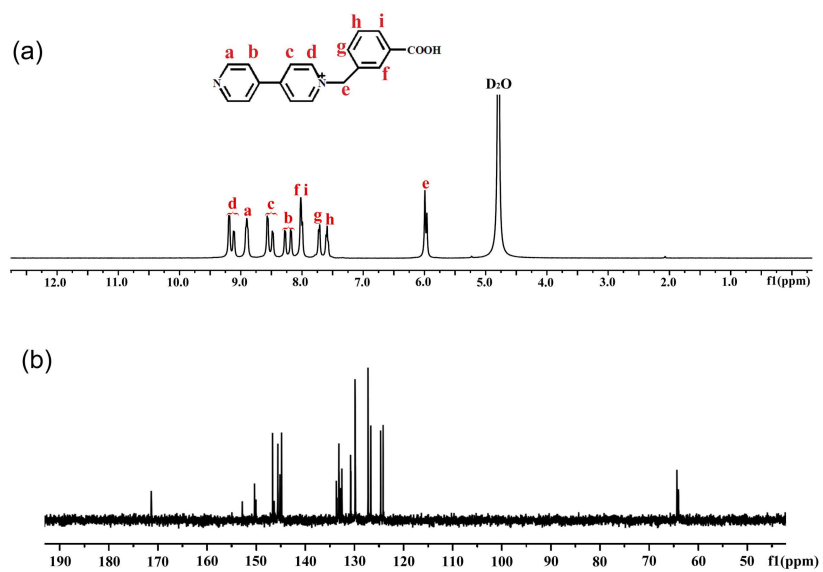


Figure S3. 2D gCOSY NMR of three viologen guests in D₂O.

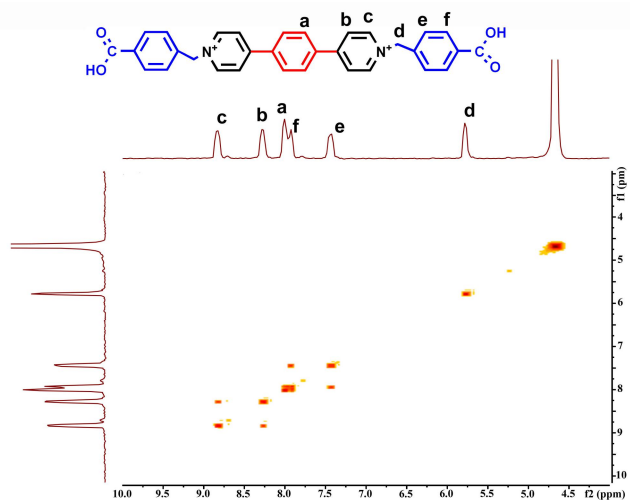
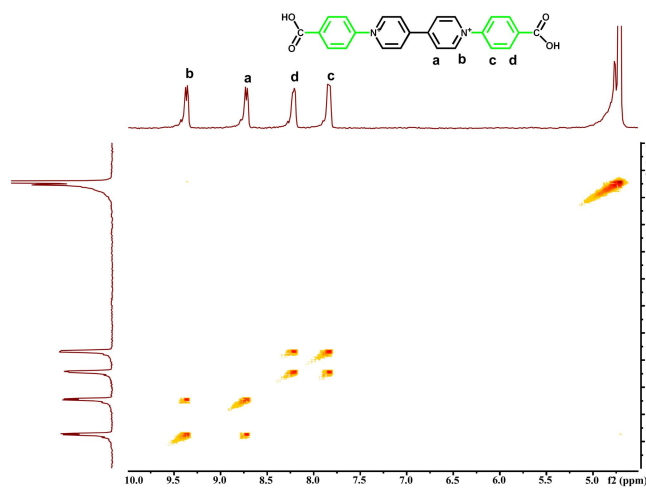
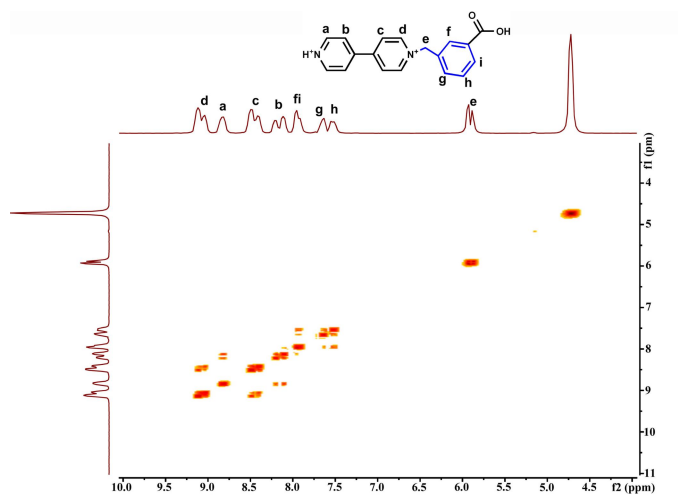


Figure S4. ^1H NMR spectra (400 MHz, D_2O) of 1^{2+} (a) in the absence and in the presence of (b) 1.53 equiv of $\beta\text{-CD}$ in D_2O at 20°C . (c) shows the ^1H NMR spectrum (400 MHz, D_2O) of $\beta\text{-CD}$ in D_2O ($5.0\text{ mmol}\cdot\text{L}^{-1}$) at 20°C .

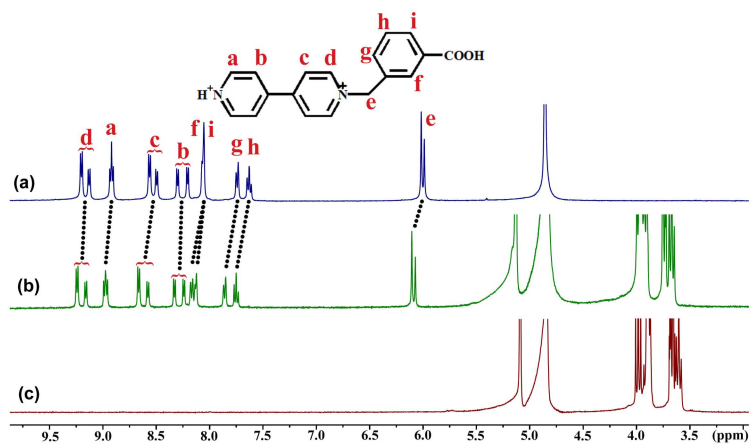


Figure S5. ^1H NMR spectra (400 MHz, D_2O) of 2^{2+} (a, $4.0\text{ mmol}\cdot\text{L}^{-1}$) in the absence and in the presence of (b) 1.70 equiv of $\beta\text{-CD}$ in D_2O at $20\text{ }^\circ\text{C}$. (c) shows the ^1H NMR spectrum (400 MHz, D_2O) of $\beta\text{-CD}$ in D_2O ($5.0\text{ mmol}\cdot\text{L}^{-1}$) at $20\text{ }^\circ\text{C}$.

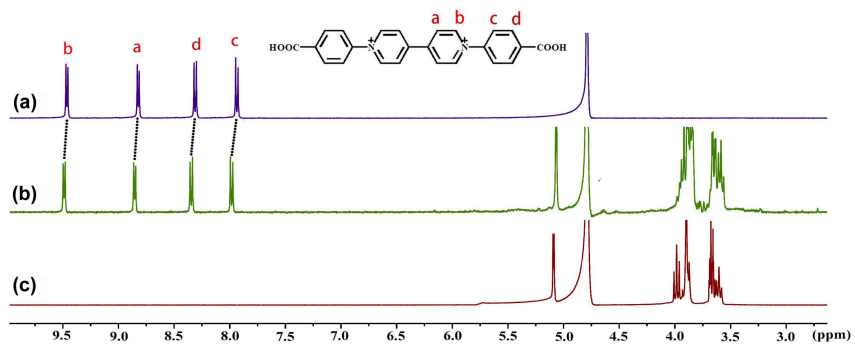


Figure S6. Photographs of the viologens $1\cdot\text{Cl}_2$, $2\cdot\text{Cl}_2$ and $3\cdot\text{Cl}_2$ before and after irradiation.

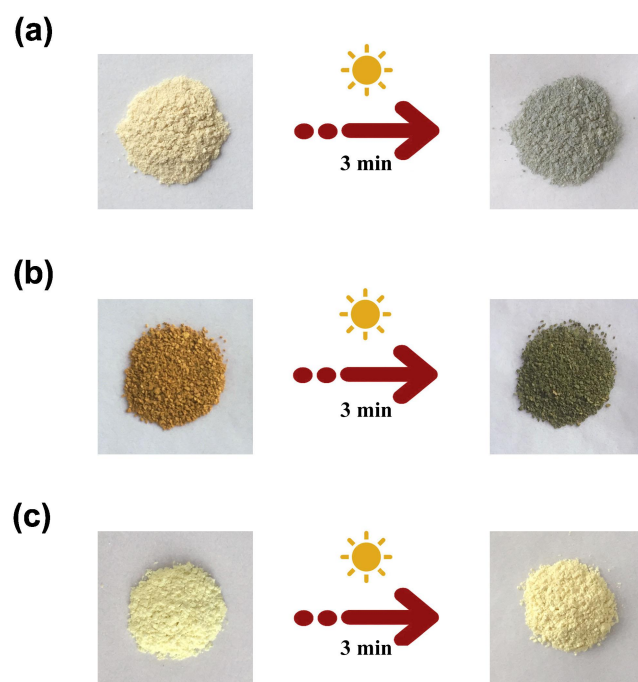


Figure S7. Photographs of surface and internal colors of the inclusion complexes after irradiation. By removing the surface materials, it can be seen that the internal colors of the inclusion complexes have not changed.

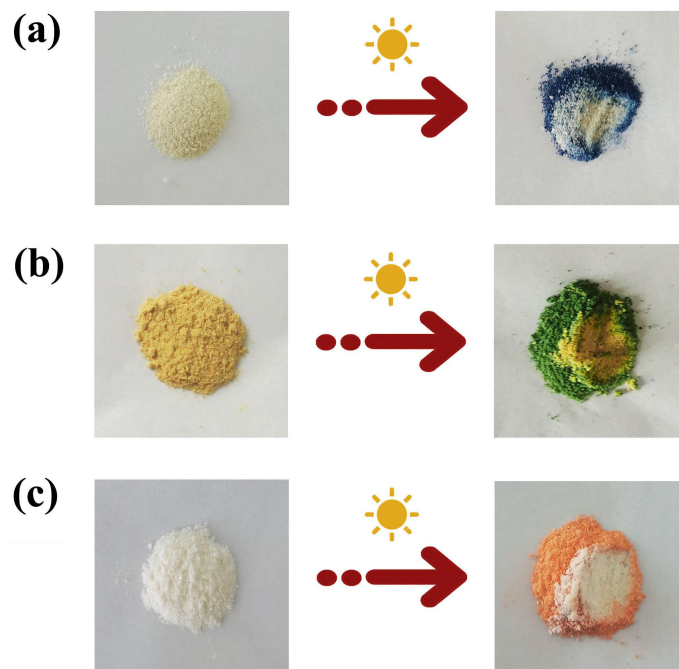


Figure S8. Electron distributions on HOMO and LUMO of the inclusion complex $1^{2+}@β\text{-CD}$.

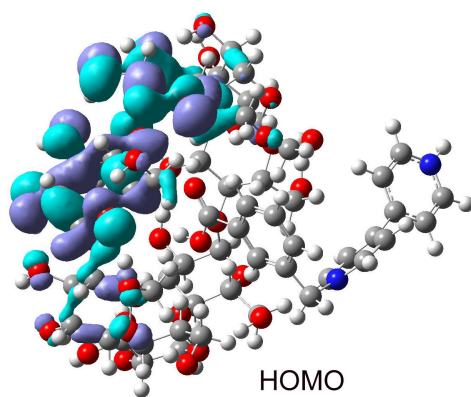
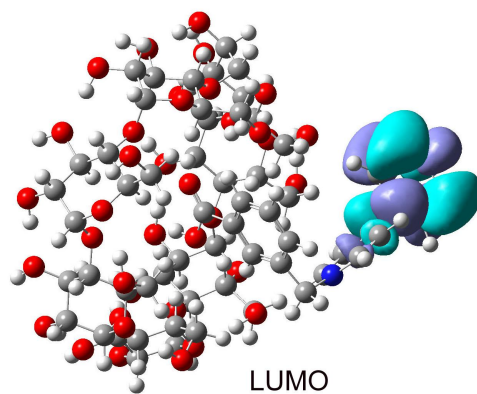


Figure S9. Electron distributions on HOMO and LUMO of the inclusion complex $2^{2+}@β\text{-CD}_2$.

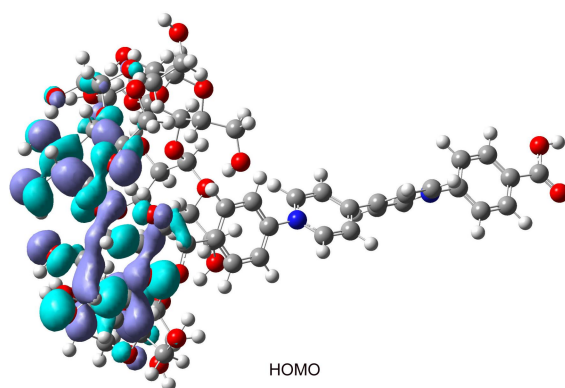
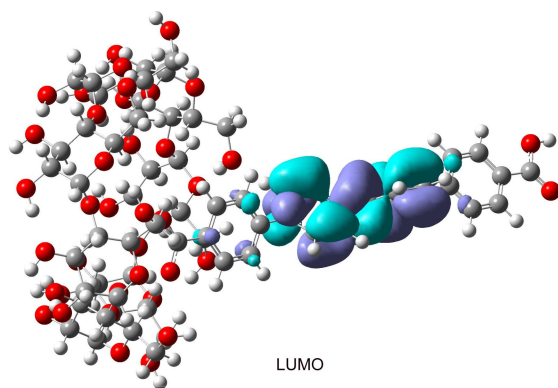


Figure S10. Electron distributions on HOMO and LUMO of the inclusion complex $3^{2+}@β$ -CD₂.

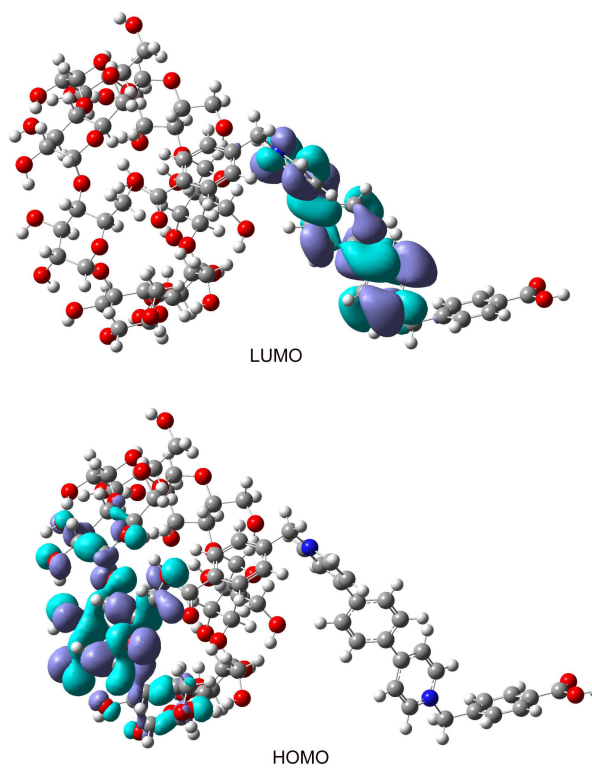


Figure S11. FI-IR spectra of the inclusion complex $1^{2+}@β\text{-CD}$ before and after irradiation.

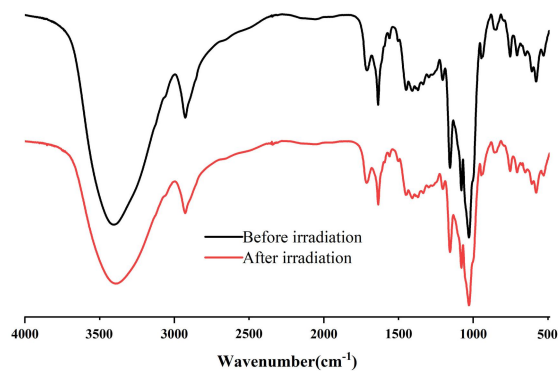


Figure S12. FI-IR spectra of the inclusion complex $2^{2+}@β\text{-CD}_2$ before and after irradiation.

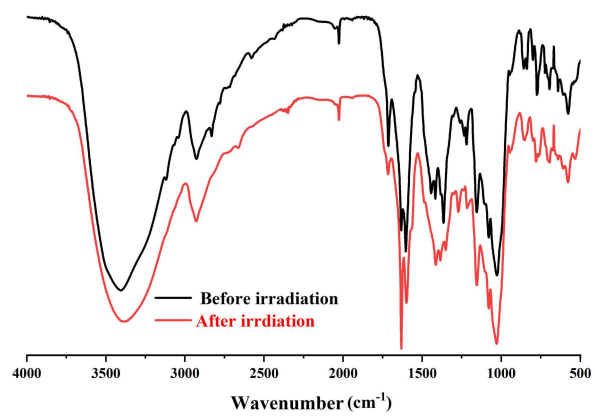


Figure S13. FI-IR spectra of the inclusion complex $3^{2+}@\beta\text{-CD}_2$ before and after irradiation.

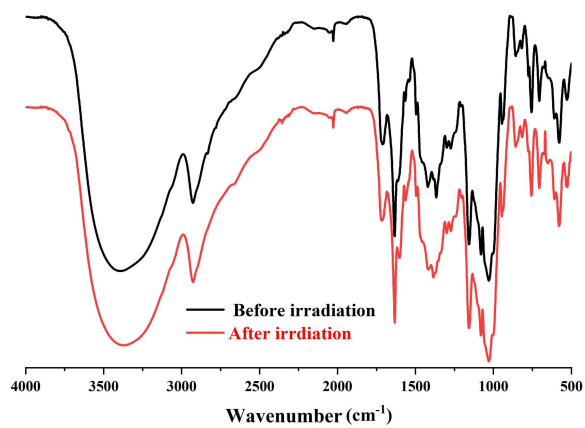


Figure S14. photomodulable fluorescence of the $1^{2+}@\beta$ -CD. (a) Photographs showing the fluorescence “on–off” switching process controlled by the photochromic process. (b) Fluorescence spectra of the solid-state $1^{2+}@\beta$ -CD changed during the light irradiation process. (c) Degree of emission intensity reduction of the solid-state $1^{2+}@ \beta$ -CD with prolonged time.

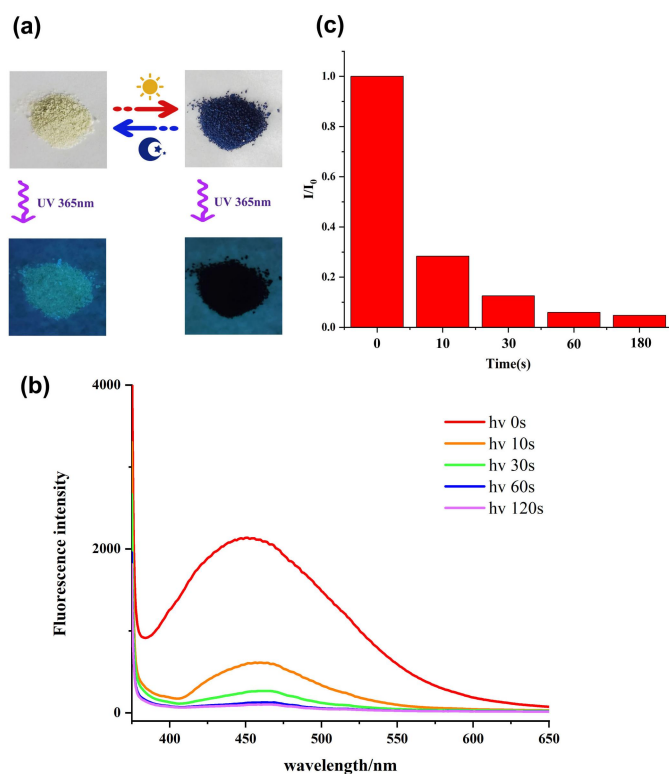


Figure S15. photomodulable fluorescence of the $2^{2+}@β\text{-CD}_2$. (a) Photographs showing the fluorescence “on–off” switching process controlled by the photochromic process. (b) Fluorescence spectra of the solid-state $2^{2+}@β\text{-CD}_2$ changed during the light irradiation process. (c) Degree of emission intensity reduction of the solid-state $2^{2+}@β\text{-CD}_2$ with prolonged time.

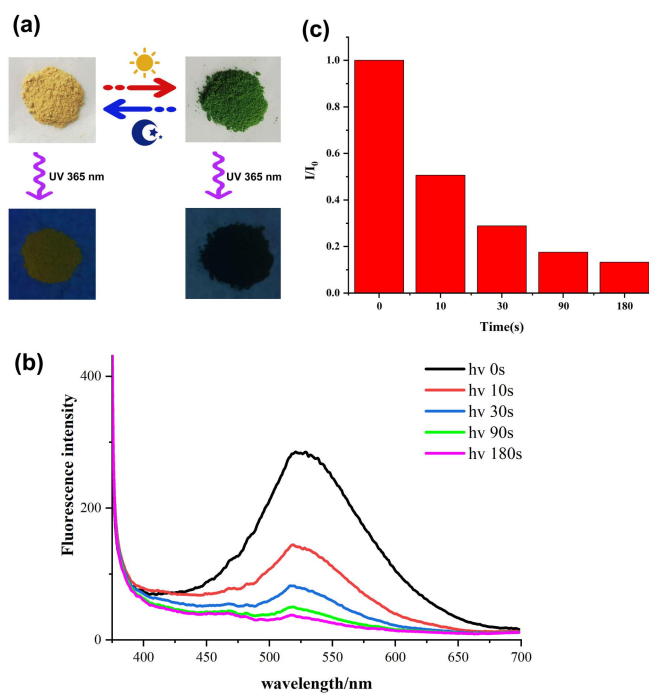


Table S1. The customized codebook 1

Combination	Letter	Combination	Letter	Combintion	Letter
111	a	211	j	311	s
112	b	212	k	312	t
113	c	213	l	313	u
121	d	221	m	321	v
122	e	222	n	322	w
123	f	223	o	323	x
131	g	231	p	331	y
132	h	232	q	332	z
133	i	233	r	333	---

Table S2. The customized codebook 2.

Combination	Letter	Combination	Letter	Combintion	Letter
333	a	233	j	133	s
332	b	232	k	132	t
331	c	231	l	131	u
323	d	223	m	123	v
322	e	222	n	122	w
321	f	221	o	121	x
313	g	213	p	113	y
312	h	212	q	112	z
311	i	211	r	111	---