

## Electronic Supplementary Information (ESI)

### Sequestration of Orange G and Methylene Blue from aqueous solutions using a Co(II) Coordination Polymer

C. R. P. Fulong<sup>a</sup> and T. R. Cook<sup>\*a</sup>

<sup>a</sup> Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, New York  
14260, USA.

\* E-mail: trcook@buffalo.edu

#### Contents

Experimental .....	2
Optical microscopy and SEM images of <i>i</i> -CoSP and <i>α</i> -CoSP .....	4
Absorption/release kinetics of <i>i</i> -CoSP and <i>α</i> -CoSP .....	5
<i>i</i> -CoSP, <i>α</i> -CoSP, and <i>r</i> -CoSP UV-Vis spectra in aqueous solutions .....	6
TGA curves of <i>i</i> -CoSP, <i>α</i> -CoSP, and <i>r</i> -CoSP before and after absorption .....	7
PXRD patterns of <i>i</i> -CoSP, <i>α</i> -CoSP, and <i>r</i> -CoSP before and after absorption .....	7
FT-IR spectra of <i>i</i> -CoSP, <i>α</i> -CoSP, and <i>r</i> -CoSP before and after absorption .....	8
XPS spectra of <i>α</i> -CoSP before and after absorption .....	9
References.....	12

#### Figures

<b>Fig. S1</b> (I) Optical microscopy and (II) SEM images of (a) <i>i</i> -CoSP and (b) <i>α</i> -CoSP. ....	3
<b>Fig. S2</b> (a) UV-Vis spectra for <i>i</i> -CoSP (top) and <i>α</i> -CoSP (bottom) absorption of aqueous dye (left: OG; right: MB); (b) First-order kinetic models for <i>i</i> -CoSP and <i>α</i> -CoSP absorption of OG and MB; (c) UV-Vis spectra for <i>α</i> -CoSP release of OG (left) and MB (right); and (d) First-order kinetic models for <i>α</i> -CoSP release of OG and MB.....	4
<b>Fig. S3</b> UV-Vis spectra of (a) <i>i</i> -CoSP and (b) <i>α</i> -CoSP in H <sub>2</sub> O; UV-Vis spectra of <i>α</i> -CoSP and <i>r</i> -CoSP in (c) water and (d) OG. ....	5
<b>Fig. S4</b> TGA curves of <i>i</i> -CoSP, <i>α</i> -CoSP, and <i>r</i> -CoSP with H <sub>2</sub> O and OG. ....	6
<b>Fig. S5</b> PXRD patterns of (a) <i>i</i> -CoSP; (b) <i>i</i> -CoSP+H <sub>2</sub> O; (c) <i>i</i> -CoSP+OG; (d) <i>α</i> -CoSP; (e) <i>α</i> -CoSP+H <sub>2</sub> O; (f) <i>r</i> -CoSP (H <sub>2</sub> O); (g) <i>α</i> -CoSP+OG; (h) <i>r</i> -CoSP (OG); and (i) simulated. ....	6
<b>Fig. S6</b> FT-IR of <i>i</i> -CoSP, <i>α</i> -CoSP, and <i>r</i> -CoSP in H <sub>2</sub> O and OG. ....	7
<b>Fig. S7</b> XPS spectra of <i>α</i> -CoSP: (a) survey; (b) Co 2p; (c) C 1s; (c) O 1s; (e) N 1s; and (f) S 2p. ....	8
<b>Fig. S8</b> XPS spectra of <i>α</i> -CoSP+H <sub>2</sub> O: (a) survey; (b) Co 2p; (c) C 1s; (c) O 1s; (e) N 1s; and (f) S 2p. ....	9
<b>Fig. S9</b> XPS spectra of <i>α</i> -CoSP+OG: (a) survey; (b) Co 2p; (c) C 1s; (c) O 1s; (e) N 1s; and (f) S 2p.....	10
<b>Fig. S10</b> XPS spectra of <i>α</i> -CoSP+MB: (a) survey; (b) Co 2p; (c) C 1s; (c) O 1s; (e) N 1s; and (f) S 2p. ....	11

#### Tables

<b>Table S1</b> Summary of first-order rate constants for of <i>i</i> -CoSP and <i>α</i> -CoSP absorption ( $k_1$ ) and release ( $k_{-1}$ ) of OG and MB. ....	7
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## Experimental

### Dye absorption

#### Crystals

The absorption of OG and MB into **CoSP** was investigated using optical microscopy.<sup>1</sup> Freshly prepared crystals immersed in the mother liquor were transferred into a glass slide. A few drops of 0.10 mM dye solution in *o*-C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub> was carefully added on the isolated crystals. The absorption of the dye was observed after a few minutes as the dye solution is concentrated by slow evaporation in air (see video S1–2).

#### Powder

The absorption of OG (and MB) into *i*-**CoSP** and **α-CoSP** were analyzed using UV-Vis spectroscopy. A stock solution of 20 mM aqueous solution of OG (26 mM of MB) were prepared. This was diluted to prepare 5 mL of 0.04 mM OG (0.01 mM MB). The absorption spectrum of the diluted solution was acquired to afford a baseline for the analysis. Then, 10 mg of *i*-**CoSP** (or **α-CoSP**) was added to the diluted dye solution. This mixture (*i*-**CoSP** + OG; *i*-**CoSP** + MB; **α-CoSP** + OG; **α-CoSP** + MB) was stirred for 30 min then left to settle. After 24 h, 3 mL aliquot of the solution was transferred into a quartz cuvette to acquire an absorption spectrum. The aliquot was then returned back to the mixture. The absorption spectrum of the solution was reacquired after 48 h. All analyses were done in triplicates.

For kinetics: Instead of stirring for 30 min, the mixture (*i*-**CoSP** + OG; *i*-**CoSP** + MB; **α-CoSP** + OG; **α-CoSP** + MB) was sonicated for 5 min, then centrifuged for 10 min. The mixture was left to stand for 5 min then 3 mL aliquot of the solution was transferred into a quartz cuvette to acquire an absorption spectrum. The aliquot was then returned back to the mixture and the sonication, centrifugation, and absorption spectrum acquisition was repeated every 20 min for 60 min.

### Dye release

#### Powder

For kinetics: The release of OG and MB from **α-CoSP** was analyzed using UV-Vis spectroscopy. Powders of **α-CoSP** + OG (or MB) from absorption experiments were air-dried. The absorption spectrum of deionized water was acquired to afford a baseline for the analysis. Then, 5 mL of deionized water was added to the air-dried powders. This mixture was sonicated for 5 min, then centrifuged for 10 min. The mixture was left to stand for 5 min then 3 mL aliquot of the solution was transferred into a quartz cuvette to acquire an absorption spectrum. The aliquot was then returned back to the mixture and the sonication, centrifugation, and absorption spectrum acquisition was repeated every 20 min for 60 min. All analyses were done in triplicates.

### Dye absorption capacity

The dye (OG and MB) concentrations, *c*, were calculated using their respective molar absorptivity coefficients (17600 M<sup>-1</sup> cm<sup>-1</sup> and 69500 M<sup>-1</sup> cm<sup>-1</sup>) at a linear range of 5–100 μM. These molar absorptivity coefficients were determined from UV-Vis absorbance measurements at 478 nm for OG and 664 nm for MB.

The equilibrium absorption capacity,  $q_e$  (mg g<sup>-1</sup>), was calculated using Equation (1),

$$q_e = \frac{(c_o - c_e)MV}{m} \quad (1)$$

where  $c_o$  is the initial concentration (mM) of dye at time 0,  $c_e$  is the equilibrium concentration (mM) of dye at time *t*, *M* is the molar mass (g mol<sup>-1</sup>) of the dye, *V* is the volume (L) of the solution, and *m* is the mass (g) of the Co sponge powder used.<sup>2</sup> All absorption capacities were calculated at 10 mg Co sponge powder loading.

### Dye absorption and release kinetics

#### Absorption

The absorption capacities,  $q_e$ , at time 0, 20, 40, and 60 min were determined from the dye absorption experiments. These were plotted and fit into a first-order kinetic model as follows (Eqn. 2):

$$\ln(q_e) = \ln(q_t) - k_1 t \quad (2)$$

where  $q_e$  (mg g<sup>-1</sup>) is the equilibrium absorption capacity,  $q_t$  (mg g<sup>-1</sup>) is the absorption capacity at time *t*,  $k_1$  (s<sup>-1</sup>) is the first-order rate constant for the absorption, and *t* (s) is the time.<sup>2</sup>

### Release

The release capacities,  $q_e$ , at time 0, 20, 40, and 60 min were determined from the dye release experiments. The equilibrium release capacity,  $q_e$  ( $mg\ g^{-1}$ ), was calculated using (Eqn. 3),

$$q_e = \frac{c_e MV}{m} \quad (3)$$

where  $c_e$  is the equilibrium concentration ( $mM$ ) of dye at time  $t$ ,  $M$  is the molar mass ( $g\ mol^{-1}$ ) of the dye,  $V$  is the volume ( $L$ ) of the solution, and  $m$  is the mass ( $g$ ) of the **CoSP** used.<sup>2</sup> All release capacities were calculated at 10 mg Co sponge powder loading. These release capacities were plotted and fit into a first-order kinetic model as shown in Eqn. 2.

### Water stability and regeneration of CoSP micro-crystallinity

The water stability and regeneration of the long-range micro-crystallinity of **CoSP** was analyzed by UV-Vis spectroscopy, PXRD, TGA, FT-IR, and XPS<sup>3</sup>.

UV-Vis spectroscopy: 10 mg of *i*-**CoSP** ( **$\alpha$ -CoSP**) was added in 5 mL of deionized water. This mixture was stirred for 30 min and left to stand for 24 h. Then the UV-Vis spectrum of the solution was acquired after 24 and 48 h.

PXRD, TGA, FT-IR, and XPS: Diffraction patterns, TGA curves, FT-IR, and XPS spectra of the air-dried powders from dye absorption and UV-Vis spectroscopy water stability experiments were measured.

Reactivation: The powders from the dye absorption and water stability experiments were reactivated following the same activation procedure mentioned previously. These reactivated powders (*r*-**CoSP**) were reanalyzed by UV-Vis spectroscopy, PXRD, TGA, and FT-IR as described above.

### Optical microscopy and SEM images of *i*-CoSP and $\alpha$ -CoSP

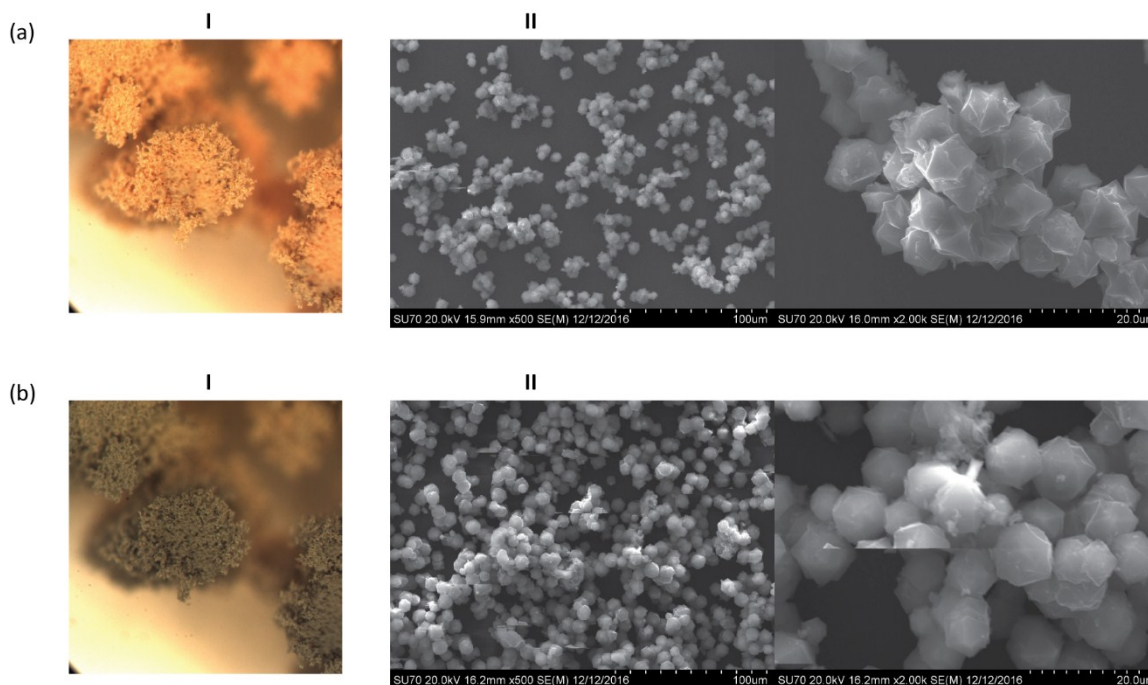
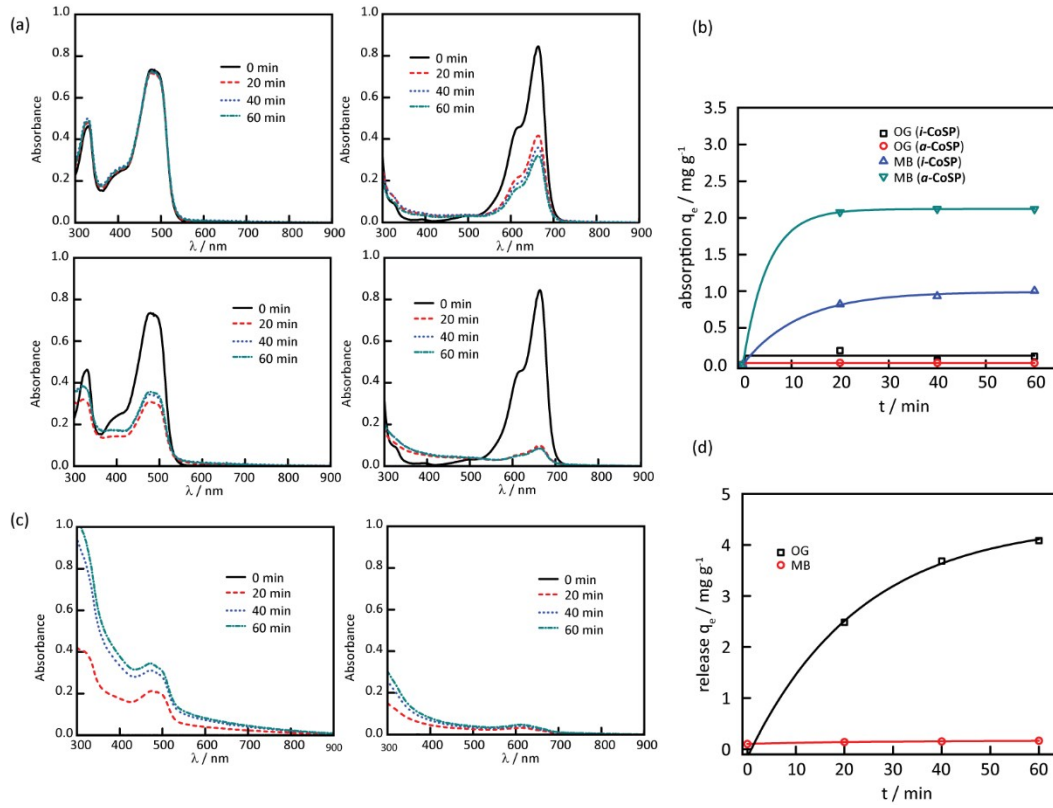


Fig. S1 (I) Optical microscopy and (II) SEM images of (a) *i*-CoSP and (b)  $\alpha$ -CoSP.

**Absorption/release kinetics of *i*-CoSP and  $\alpha$ -CoSP**



**Fig. S2** (a) UV-Vis spectra for *i*-CoSP (top) and  $\alpha$ -CoSP (bottom) absorption of aqueous dye (left: OG; right: MB); (b) First-order kinetic models for *i*-CoSP and  $\alpha$ -CoSP absorption of OG and MB; (c) UV-Vis spectra for  $\alpha$ -CoSP release of OG (left) and MB (right); and (d) First-order kinetic models for  $\alpha$ -CoSP release of OG and MB.

*i*-CoSP,  $\alpha$ -CoSP, and *r*-CoSP UV-Vis spectra in aqueous solutions

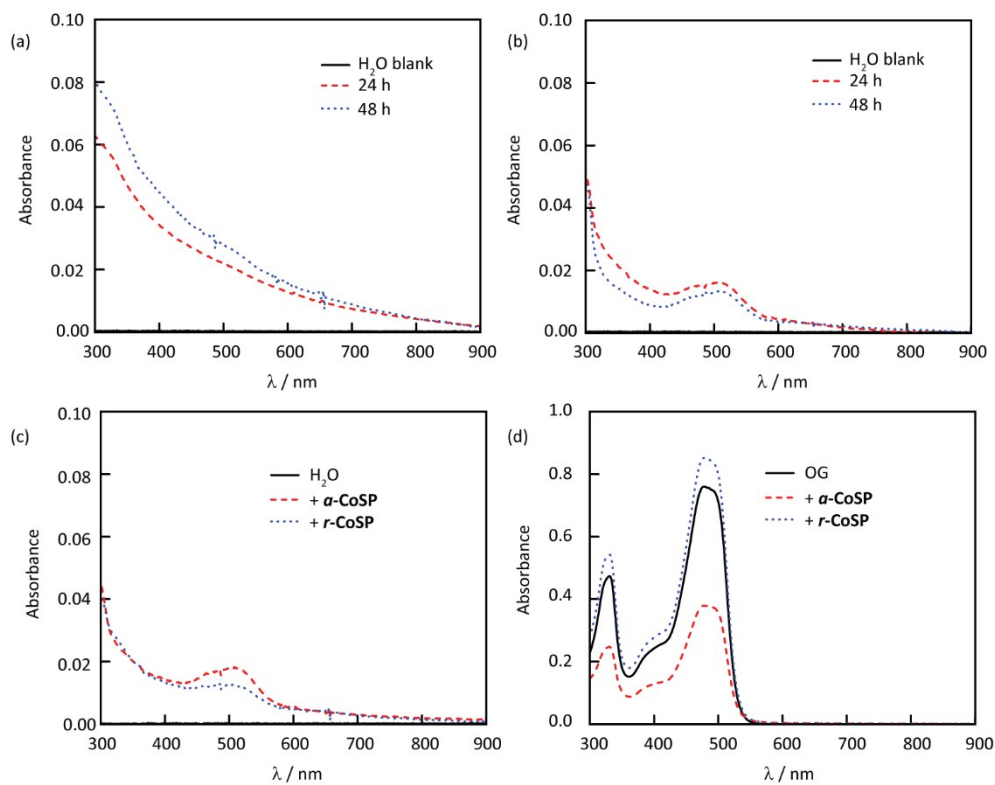


Fig. S3 UV-Vis spectra of (a) *i*-CoSP and (b)  $\alpha$ -CoSP in H<sub>2</sub>O; UV-Vis spectra of  $\alpha$ -CoSP and *r*-CoSP in (c) water and (d) OG.

TGA curves of *i*-CoSP,  $\alpha$ -CoSP, and *r*-CoSP before and after absorption

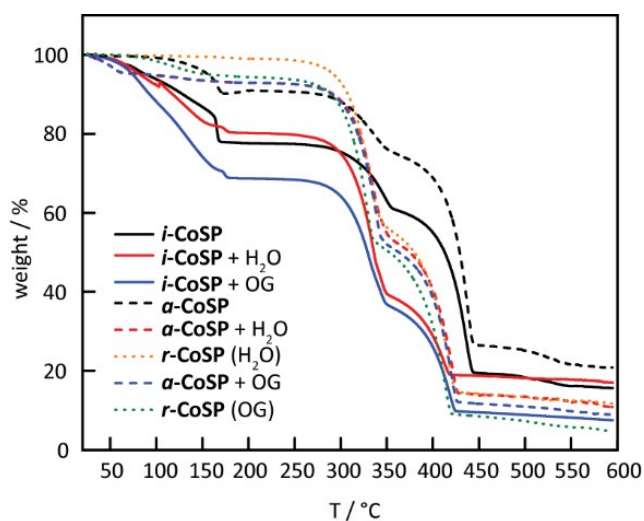


Fig. S4 TGA curves of *i*-CoSP,  $\alpha$ -CoSP, and *r*-CoSP with H<sub>2</sub>O and OG.

PXRD patterns of *i*-CoSP,  $\alpha$ -CoSP, and *r*-CoSP before and after absorption

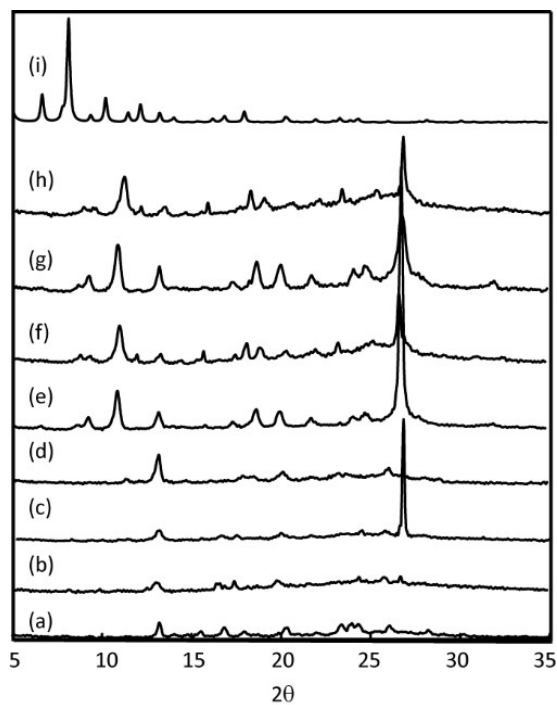


Fig. S5 PXRD patterns of (a) *i*-CoSP; (b) *i*-CoSP+H<sub>2</sub>O; (c) *i*-CoSP+OG; (d)  $\alpha$ -CoSP; (e)  $\alpha$ -CoSP+H<sub>2</sub>O; (f) *r*-CoSP (H<sub>2</sub>O); (g)  $\alpha$ -CoSP+OG; (h) *r*-CoSP (OG); and (i) simulated.

FT-IR spectra of *i*-CoSP,  $\alpha$ -CoSP, and *r*-CoSP before and after absorption

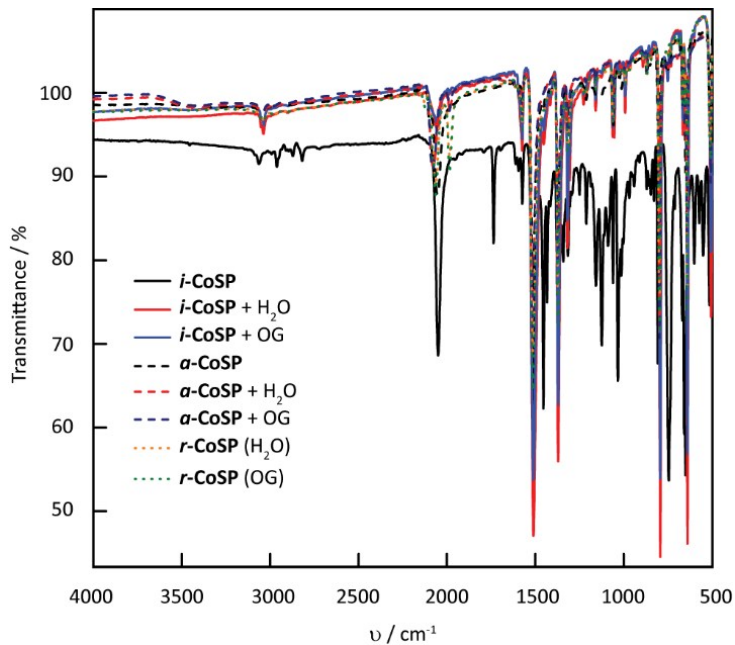


Fig. S6 FT-IR of *i*-CoSP,  $\alpha$ -CoSP, and *r*-CoSP in H<sub>2</sub>O and OG.

Table S1 Summary of first-order rate constants for of *i*-CoSP and  $\alpha$ -CoSP absorption ( $k_1$ ) and release ( $k_{-1}$ ) of OG and MB.

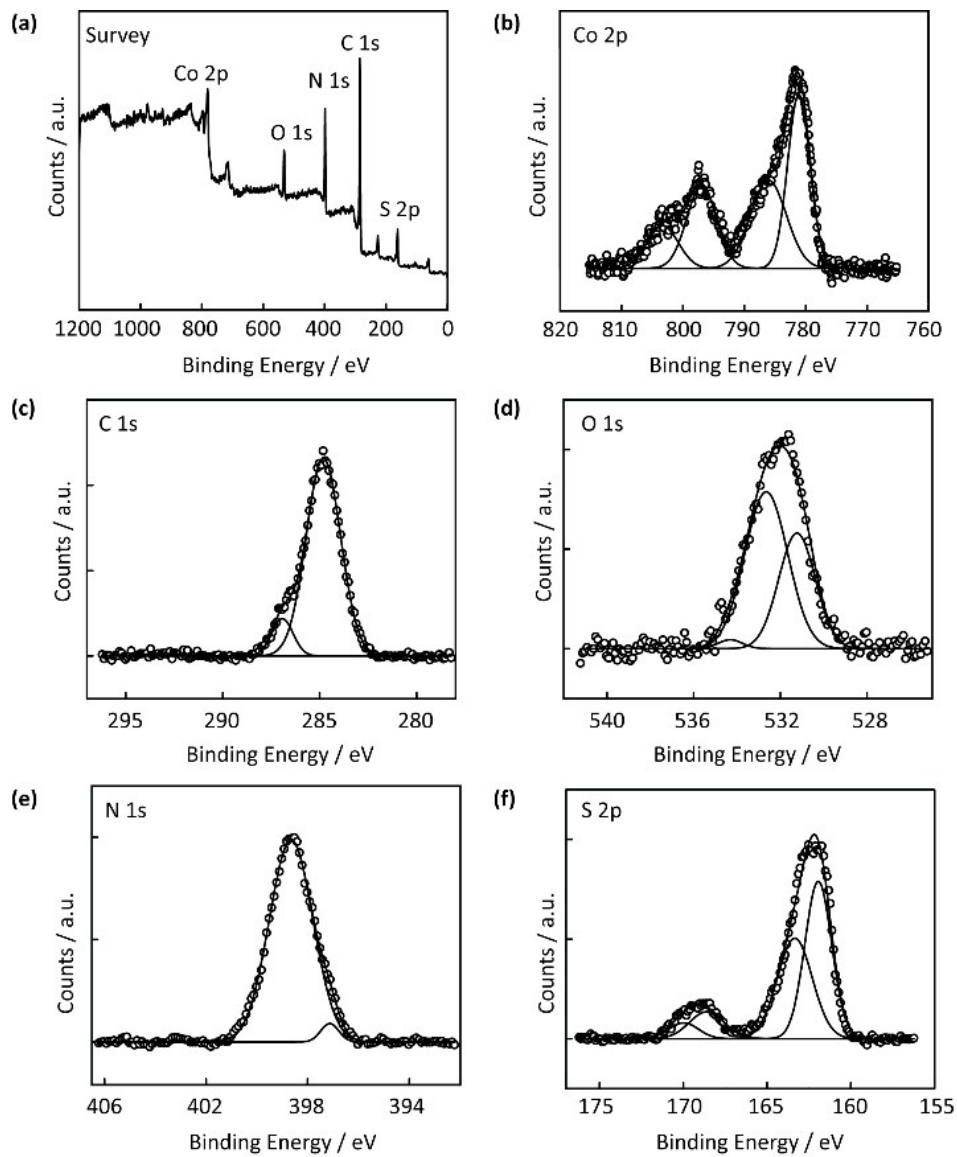
Dye	Co sponge powder	R <sup>2</sup> *	1/ $k_1$ , s*	$k_1$ , s <sup>-1</sup>	$k_{-1}$ , s <sup>-1</sup>	
Absorption	OG	<i>i</i> -CoSP	-0.45	0.09(**)	12	-
		$\alpha$ -CoSP	0.90223	0.42(**)	2	-
	MB	<i>i</i> -CoSP	0.99447	12(2)	0.09	-
		$\alpha$ -CoSP	1	5.09(8)	0.20	-
Release	OG	$\alpha$ -CoSP	0.99893	23(2)	-	0.04
	MB	$\alpha$ -CoSP	-	-	-	-

\* modeled parameters

\*\* standard error greater than reported value

## XPS spectra of $\alpha$ -CoSP before and after absorption

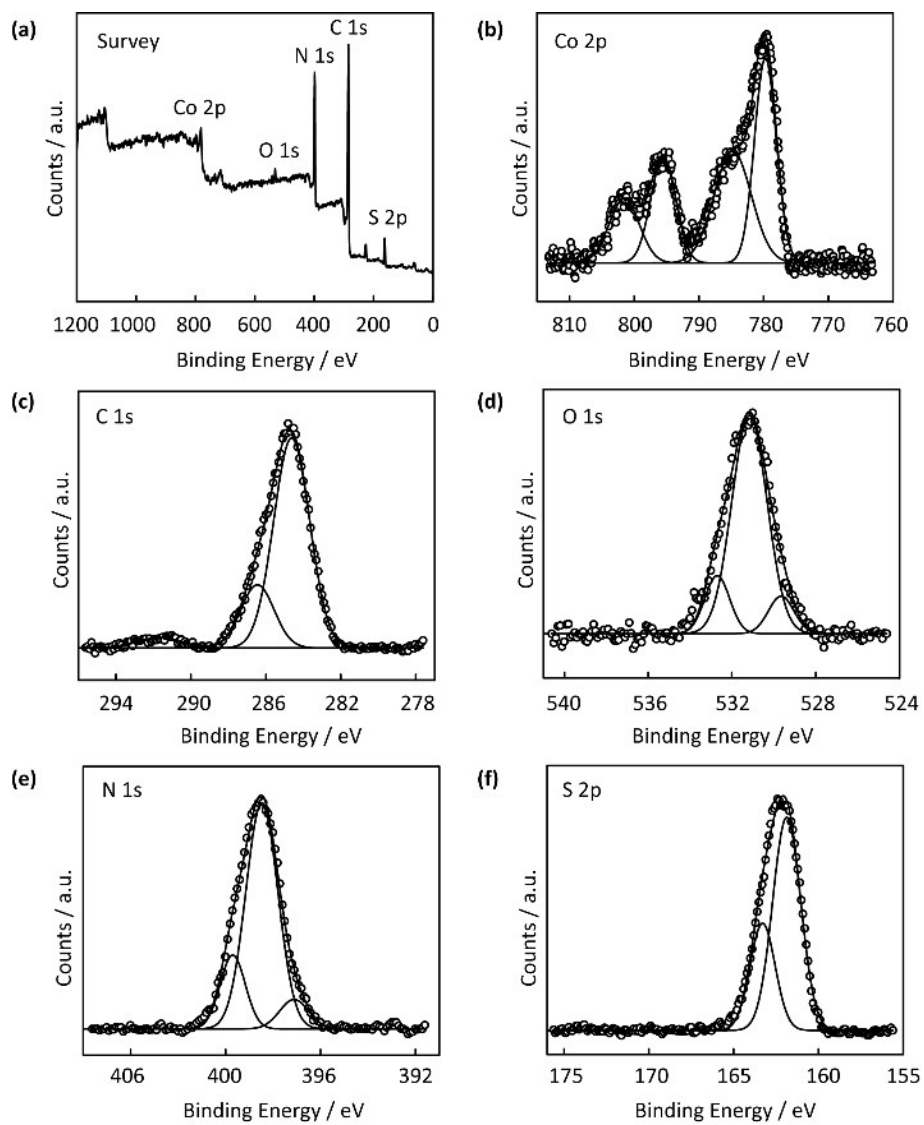
Activated CoSP powder:



**Fig. S7** XPS spectra of  $\alpha$ -CoSP: (a) survey; (b) Co 2p; (c) C 1s; (d) O 1s; (e) N 1s; and (f) S 2p.

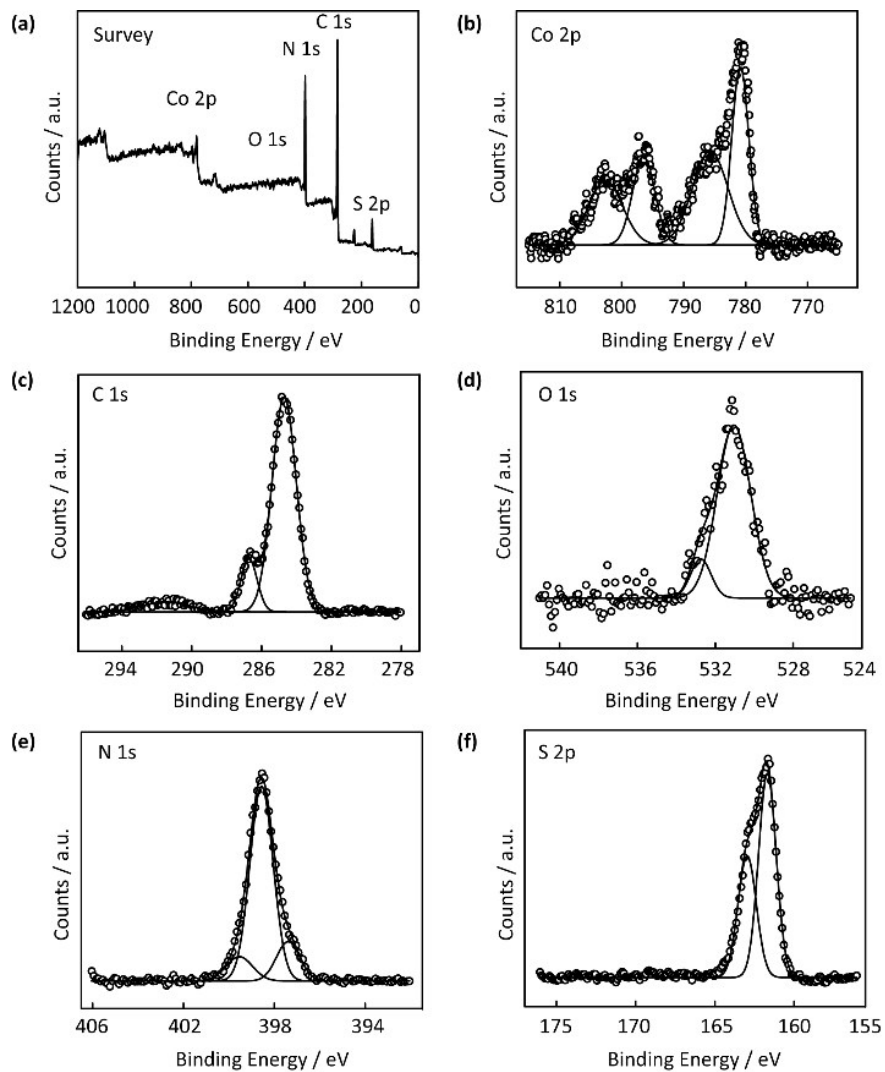


Activated CoSP in water:



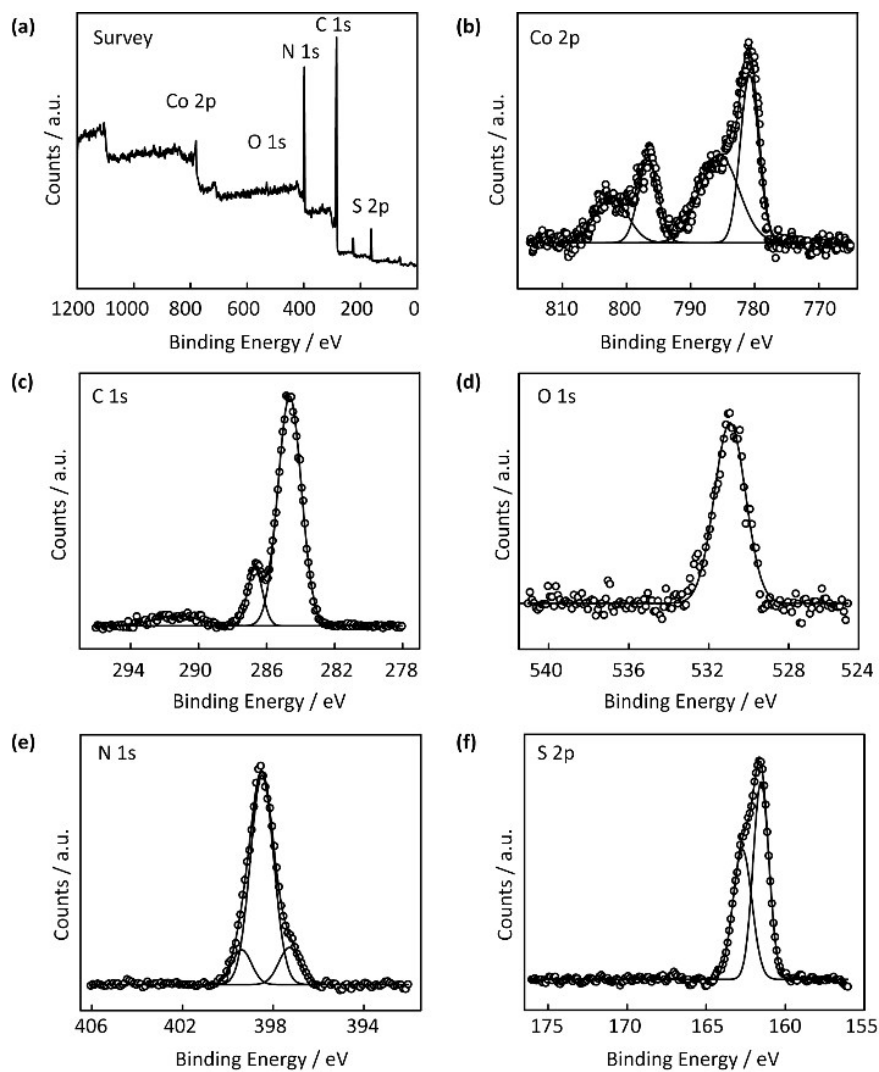
**Fig. S8** XPS spectra of  $\alpha$ -CoSP+H<sub>2</sub>O: (a) survey; (b) Co 2p; (c) C 1s; (d) O 1s; (e) N 1s; and (f) S 2p.

Activated CoSP in aqueous OG:



**Fig. S9** XPS spectra of  $\alpha$ -CoSP+OG: (a) survey; (b) Co 2p; (c) C 1s; (d) O 1s; (e) N 1s; and (f) S 2p.

Activated CoSP in aqueous MB:



**Fig. S10** XPS spectra of  $\alpha$ -CoSP+MB: (a) survey; (b) Co 2p; (c) C 1s; (d) O 1s; (e) N 1s; and (f) S 2p.

## References

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2. Z.-P. Qi, J.-M. Yang, Y.-S. Kang, F. Guo and W.-Y. Sun, *Dalton Trans.*, 2016, **45**, 8753-8759.
3. J. Jiang, L. Huang, X. Liu and L. Ai, *ACS Appl. Mater. Interfaces*, 2017, **9**, 7193-7201.