

## Supporting Information

### Dynamic Investigation of **Gas-releasing** Chemical Reaction through Photonic

#### Crystal

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### Experimental Section

#### *Materials*

Silica ( $\text{SiO}_2$ ) spheres were purchased from Nanjing Caina Corporation. Hydrogen peroxide ( $\text{H}_2\text{O}_2$ ), methylbenzene and sulfuric acid ( $\text{H}_2\text{SO}_4$ ) were obtained from Beijing Chemical Corporation. Potassium iodide (KI), benzoic acid, sulfanilamide and cephalexin were purchased from Beijing Innochem Corporation. Chlorinated polypropylene (CPP) was obtained from Wuhan Yuancheng Corporation. Ferrous sulfate ( $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ ), iron sulfate ( $\text{Fe}_2(\text{SO}_4)_3$ ) and aluminium trichloride ( $\text{AlCl}_3$ ) were purchased from Alfa.

#### *Self-assembly of PC*

The  $\text{SiO}_2$  spheres were assembled into PC on glass slides by using the vertical deposition method.<sup>[1]</sup> First, the glass slides were cleaned ultrasonically in distilled water, acetone and ethanol for 30 min each. Then, the cleaned glass slides were placed vertically into cylindrical vessels. The  $\text{SiO}_2$  suspension was added to the vessel and self-assembled for 48 h to form  $\text{SiO}_2$  PC in an incubator. Concentration of  $\text{SiO}_2$  spheres is 0.5 wt. % in 1 mL of water and 4 mL of ethanol. Experimental condition is at a stable temperature of 60 °C and relatively humidity of 60 %.

#### *Materials Characterizations and Measurement of Dynamic Reflection Spectra of PC*

Scanning electron microscopy (SEM) images were obtained from JSM-7500F

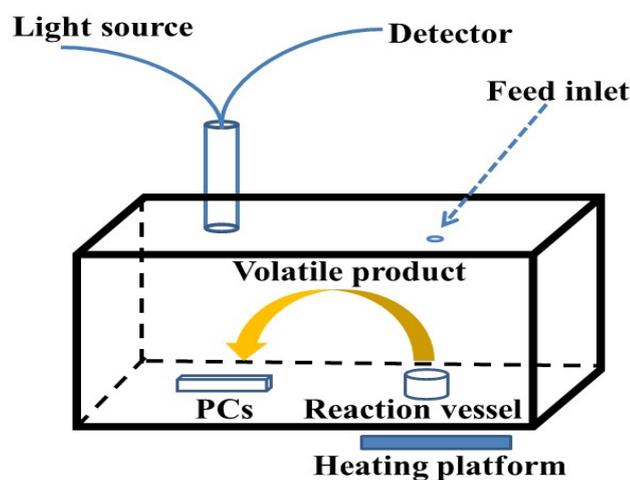
(Japan). The reflection spectra of PC in normal incidence were recorded using a R1 fiber optic spectrometer (Ideaoptics, China). PC was placed in a sealed cuboid ( $l \times w \times h = 75 \text{ mm} \times 45 \text{ mm} \times 20 \text{ mm}$ ) with a hole as a sensor to monitor chemical reaction (Figure S1). The cuboid was dried by  $\text{N}_2$ . Dynamic reflection spectra of PC were tested at a constant temperature of  $25 \text{ }^\circ\text{C}$ .

Typically,  $0.2 \text{ mL}$  of  $\text{H}_2\text{O}_2$  aqueous solution (4%) was injected into the small reaction vessel ( $0.6 \text{ mL}$ ) through the hole using a small syringe. Then  $0.2 \text{ mL}$  of KI ( $0.2 \text{ mol/L}$ ) was fed to the  $\text{H}_2\text{O}_2$  aqueous solution. The in situ reflection spectra of the PC were automatically recorded every  $5 \text{ s}$  in the next  $45 \text{ min}$  by the R1 spectrophotometer at normal incidence.  $\text{H}_2\text{O}_2$  reacted with KI and generated  $\text{O}_2$ , PC absorbed ceaselessly the  $\text{O}_2$  as the chemical reaction gone on, causing a corresponding red shift. Chemicals reaction process was detected according to change of the stopband shifts of the PC with time.

$\text{AlCl}_3$  as catalyst was fed to the small reaction vessel.  $0.5 \text{ mL}$  of CPP in methylbenzene solution ( $0.3 \text{ g/mL}$ ) was injected into the small reaction vessel through the hole using a syringe. CPP reacted with methylbenzene and generated hydrogen chloride (HCl), PC absorbed the HCl as the chemical reaction gone on, causing a corresponding red shift. The cuboid is put on heating platform to achieve different reaction temperatures. The heating platform can support a constant temperature of  $35$  or  $45 \text{ }^\circ\text{C}$ . Chemicals reaction process was detected according to change of the stopband shifts of the PC with time.

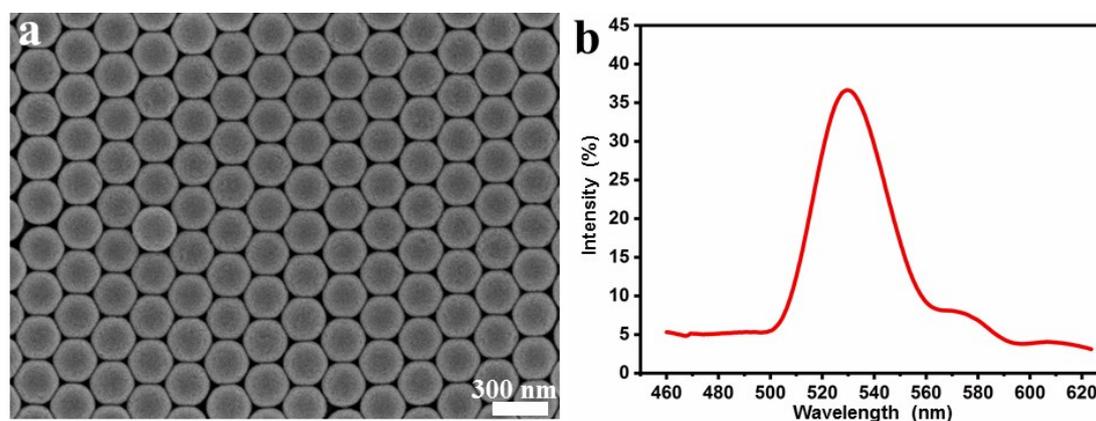
$0.3 \text{ mL}$  of benzoic acid ( $1.0 \text{ g/L}$ ),  $0.04 \text{ mL}$  of  $\text{FeSO}_4$  ( $0.032 \text{ mol/L}$ ) and  $0.02 \text{ mL}$  of  $\text{H}_2\text{SO}_4$  ( $0.001 \text{ mol/L}$ ) were mixed. Then the  $0.36 \text{ mL}$  of mixed solution was injected into the small reaction vessel through the hole using a syringe.  $0.1 \text{ mL}$  of  $\text{H}_2\text{O}_2$  aqueous solution (1 %) was added to the mixed solution. Benzoic acid was

oxidative degradation and generated  $\text{CO}_2$ . PC absorbed the  $\text{CO}_2$  as the chemical reaction gone on. In situ reflection spectra of the PC were automatically recorded every 5 s in the next 15 min by the R1 spectrophotometer at normal incidence.



**Figure S1** Schematic illustration of the system to monitor micro-chemical reaction through PC.

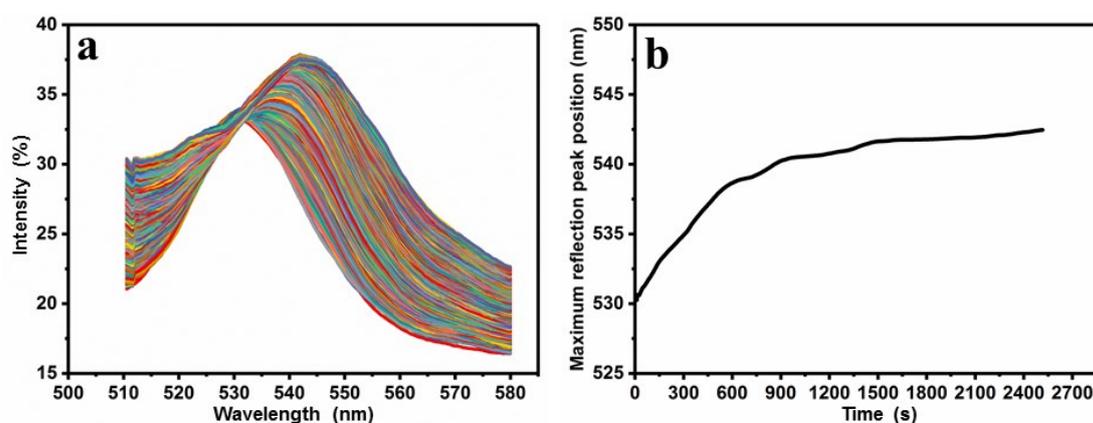
### Experimental Result Section



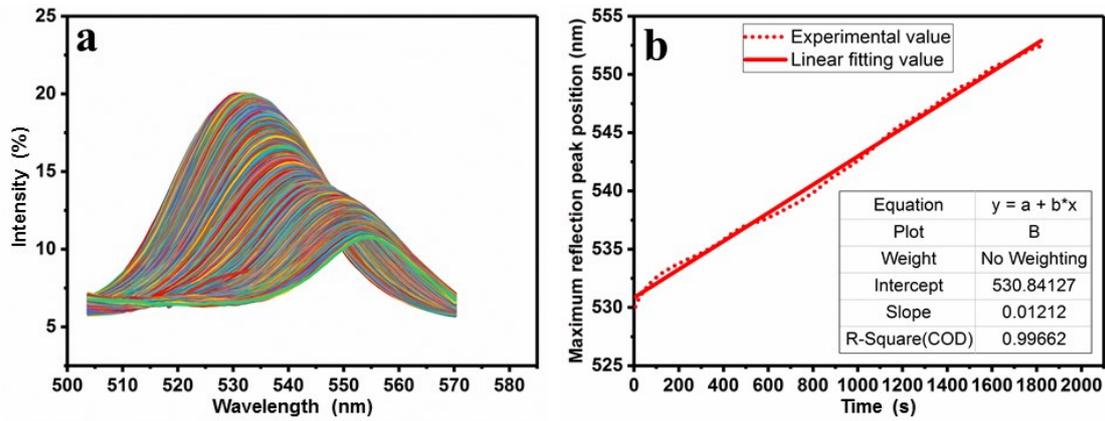
**Figure S2** SEM image of PC from 235 nm of  $\text{SiO}_2$  spheres. b) Reflection spectrum of the  $\text{SiO}_2$  PC. The  $\text{SiO}_2$  spheres are assembled in a face-centered cubic arrangement with the close-packed plane oriented parallel onto substrate, presenting a highly ordered hexagonal structure. The average diameter of the  $\text{SiO}_2$  spheres is 235 nm. The corresponding reflection peak of the  $\text{SiO}_2$  PC is located at 530 nm.

**Table S1** The  $t_{\text{balance}}$ , stopband shifts and the average speeds of reflection peak position shift for PC response to chemical reactions under different concentrations of  $\text{H}_2\text{O}_2$  and KI. With increase of concentration of  $\text{H}_2\text{O}_2$ , the stopband shifts and  $v'$  increase obviously. With increase of concentration of KI,  $t_{\text{balance}}$  decreases obviously, leading to the increase of  $v'$ .

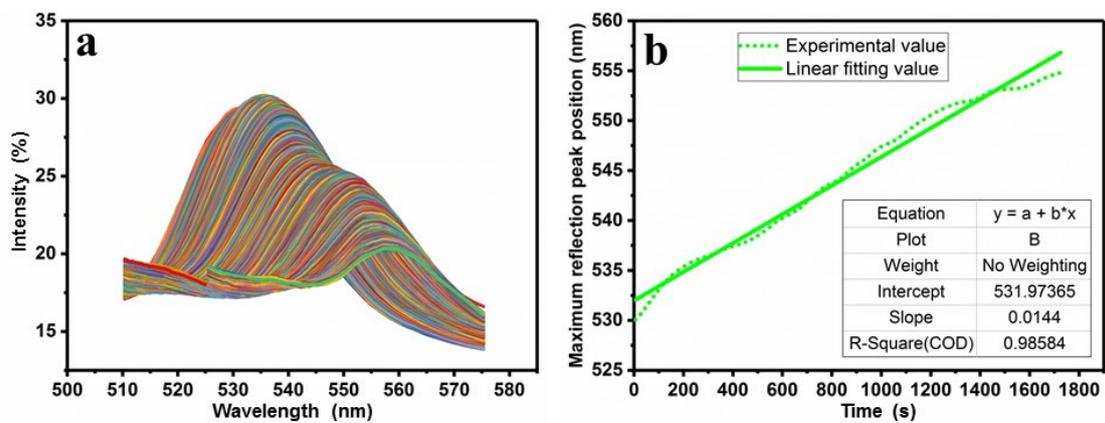
Experimental number	Ratio of $\text{H}_2\text{O}_2$ (%)	KI (mol/L)	$t_{\text{balance}}$ (s)	Stopband shifts (nm)	$v'$ ( $\times 10^{-3}\text{nm/s}$ )
1	2	0	-	-	-
2	2	0.1	1820	22.0	12.1
3	4	0.1	1725	24.8	14.4
4	6	0.1	1420	26.1	18.4
5	4	0.2	1405	22.1	15.7
6	4	0.3	850	19.2	22.6



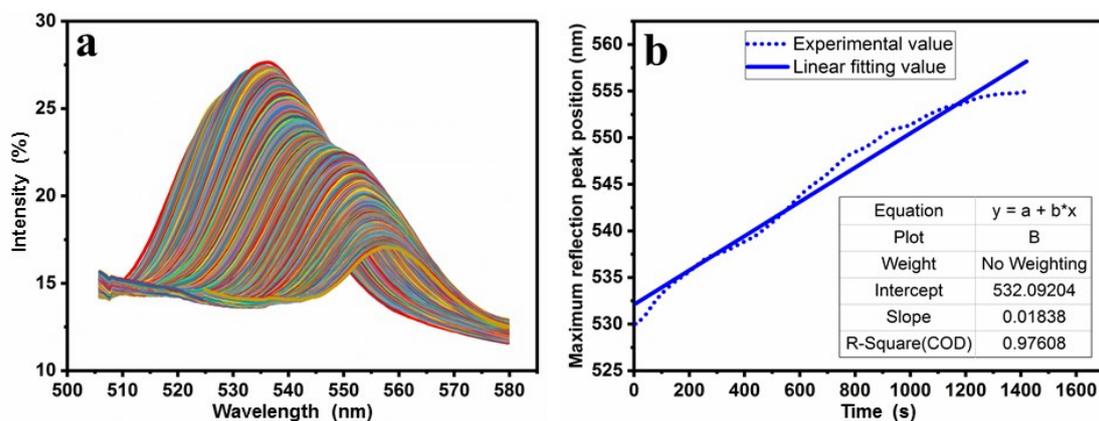
**Figure S3** a) Reflection spectra of PC response to  $\text{H}_2\text{O}_2$  aqueous solution at experiment 1. b) The change curve of the corresponding maximum reflection peak position of PC with time. The stopbands have a little red shift as the solvent volatilizes.



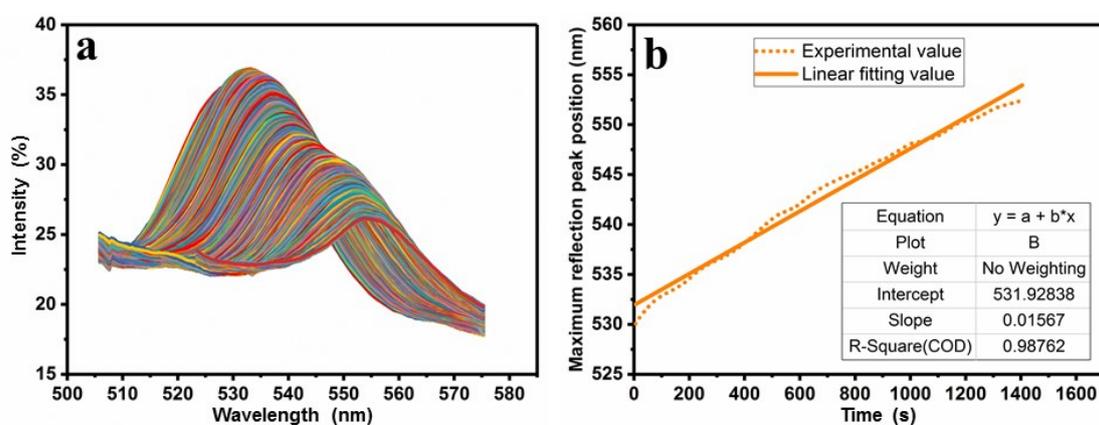
**Figure S4** a) Reflection spectra of PC response to chemical reaction at experiment 2. b) The experimental value and linear fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99, indicating that the linear fitting is reasonable.



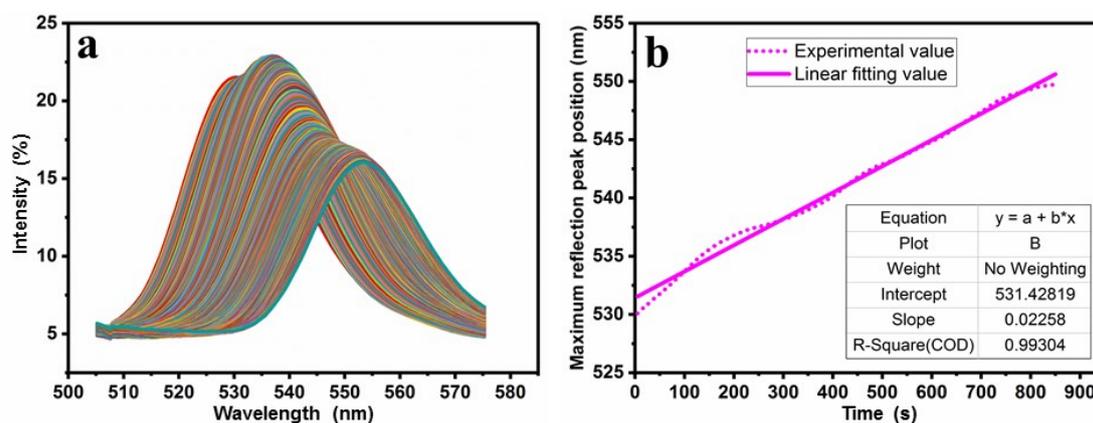
**Figure S5** a) Reflection spectra of PC response to chemical reaction at experiment 3. b) The experimental value and linear fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.98.



**Figure S6** a) Reflection spectra of PC response to chemical reaction at experiment 4.  
 b) The experimental value and linear fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.976.



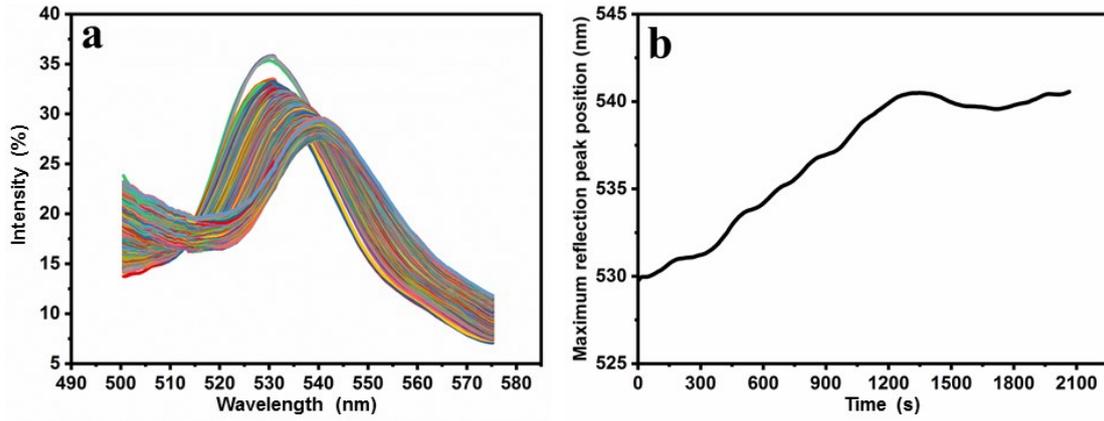
**Figure S7** a) Reflection spectra of PC response to chemical reaction at experiment 5.  
 b) The experimental value and linear fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.98.



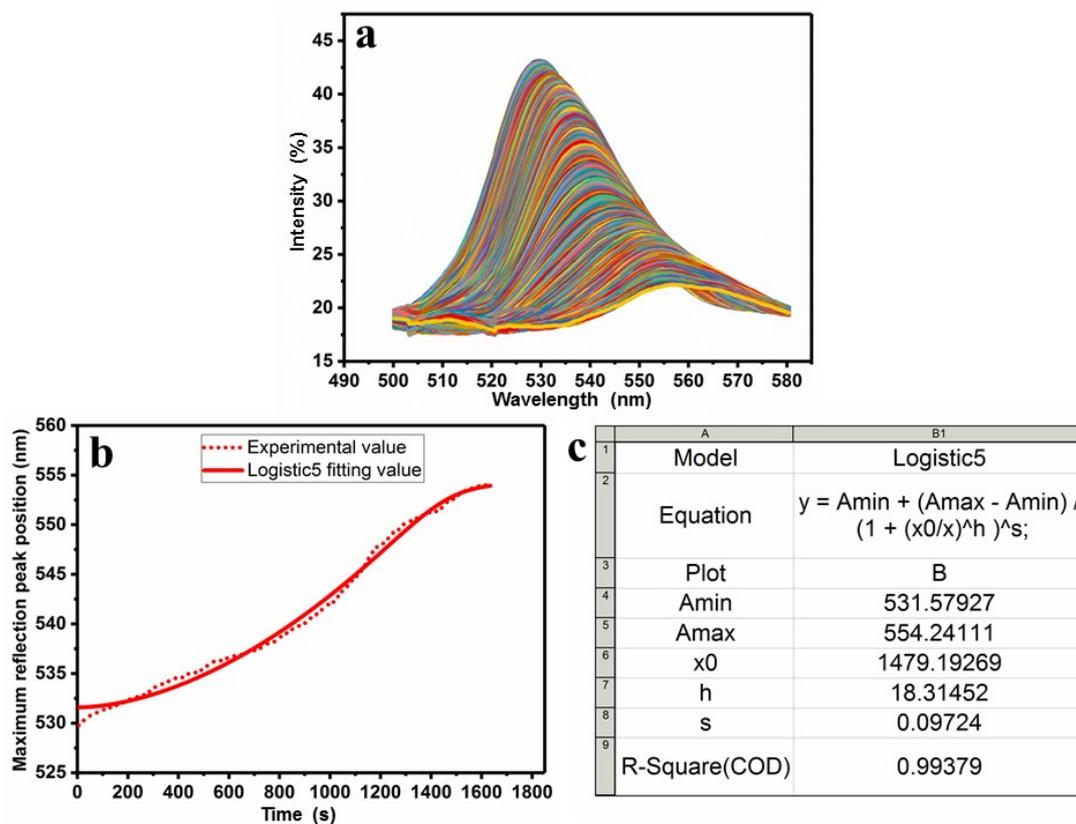
**Figure S8** a) Reflection spectra of PC response to chemical reaction at experiment 6. b) The experimental value and linear fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.

**Table S2** The  $t_{\text{balance}}$ , stopband shifts and the average speeds of reflection peak position shift of PC response to chemical reactions under different ratios of  $\text{AlCl}_3$  and reaction temperatures. With increase of amount of  $\text{AlCl}_3$  and reaction temperatures, the  $v'$  increases obviously.

Experimental number	T (°C)	CPP (g/mL)	Ratio of $\text{AlCl}_3$ (wt %)	$t_{\text{balance}}$ (s)	Stopband shifts (nm)	$v'$ ( $\times 10^{-3}$ nm/s)
7	25	0.3	0	-	-	-
8	25	0.3	5	1585	23.9	15.1
9	25	0.3	10	1150	24.6	21.4
10	25	0.3	15	900	23.5	26.1
11	35	0.3	5	785	20.6	26.2
12	45	0.3	5	530	17.4	32.8

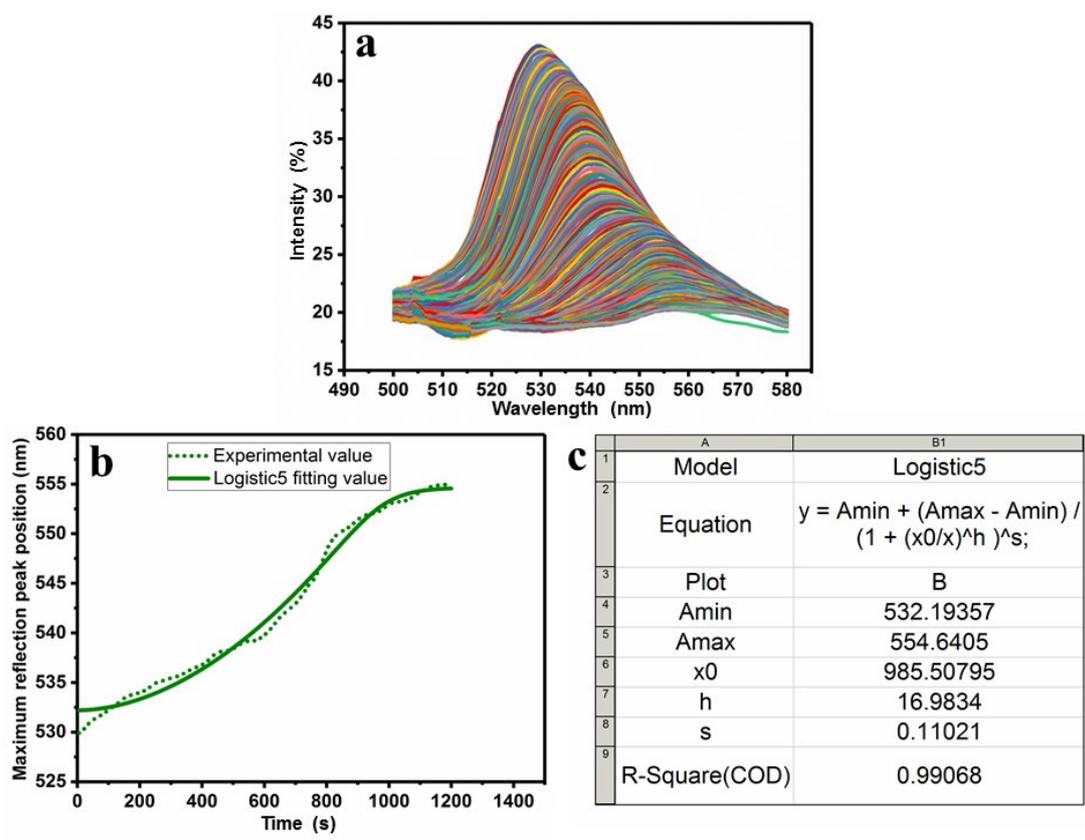


**Figure S9** a) Reflection spectra of PC response to CPP methylbenzene solution at experiment 7. b) The change curve of the corresponding maximum reflection peak position of PC with time. The stopbands have a little red shift as methylbenzene volatilizes.

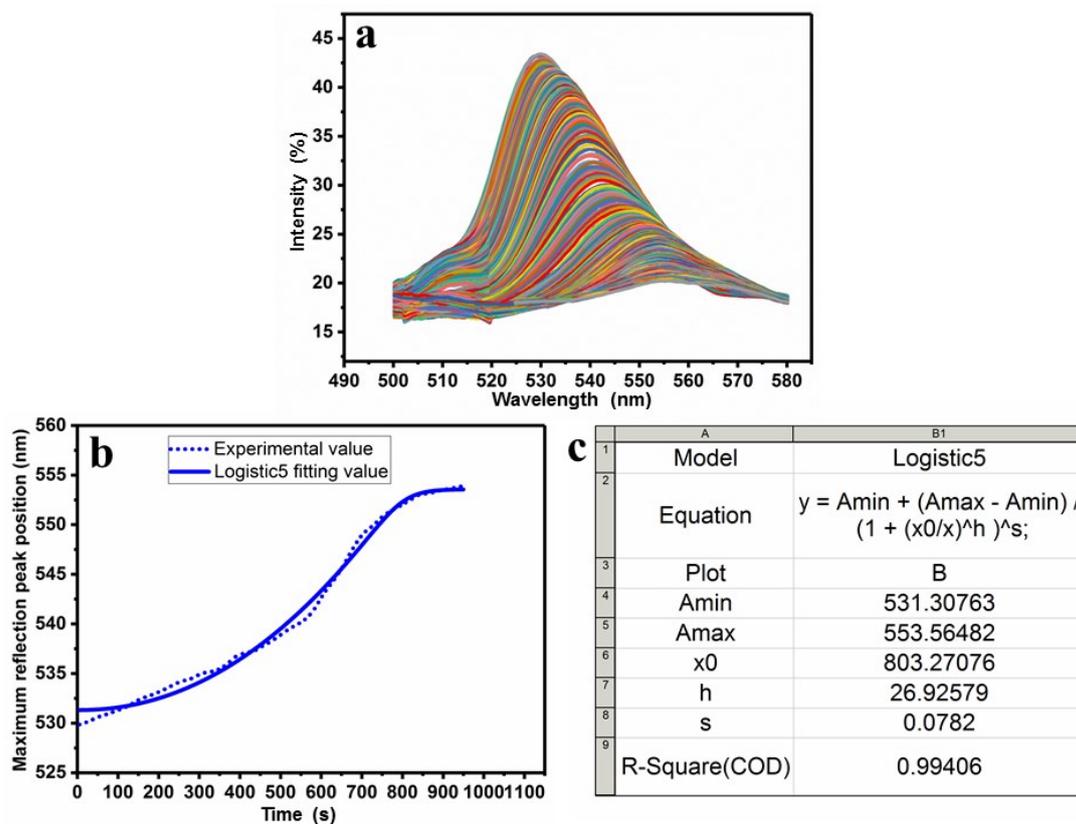


**Figure S10** a) Reflection spectra of PC response to chemical reaction at experiment 8.

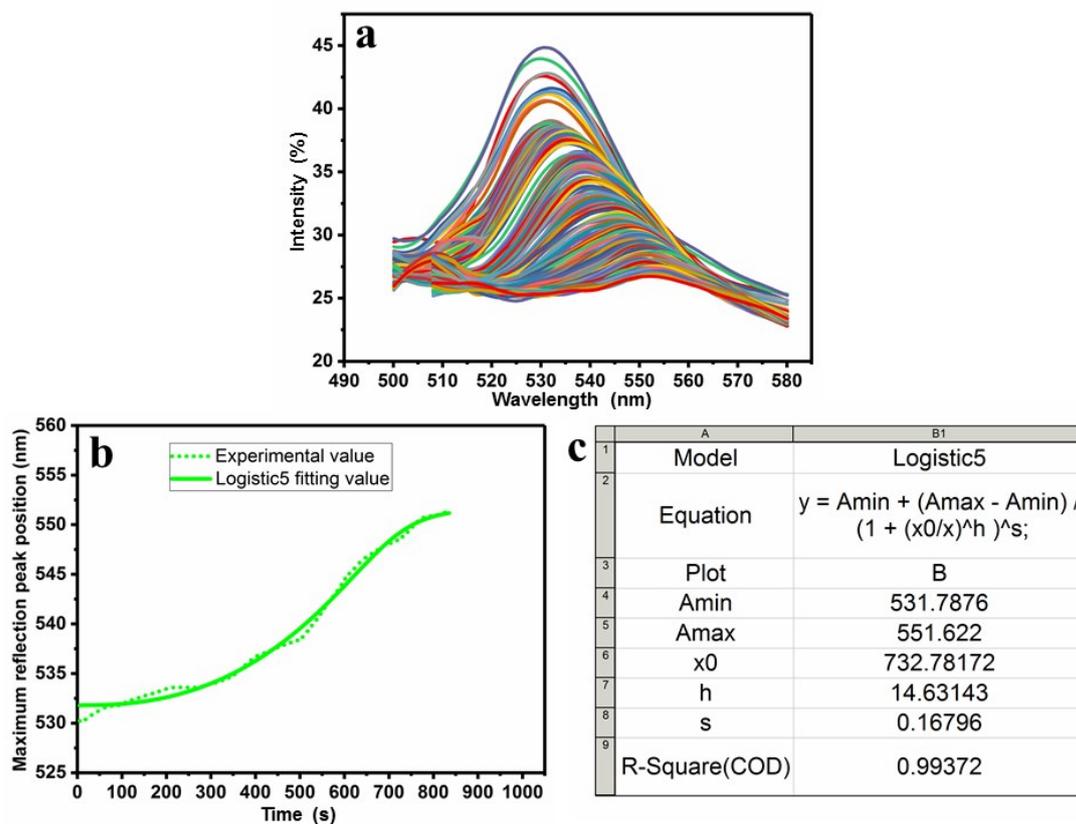
b) The experimental value and logistic5 fitting value of the corresponding maximum reflection peak position of PC with time including in  $t_{balance}$  and extra 50 s. R-Square is over 0.99, indicating that the logistic5 fitting is reasonable.



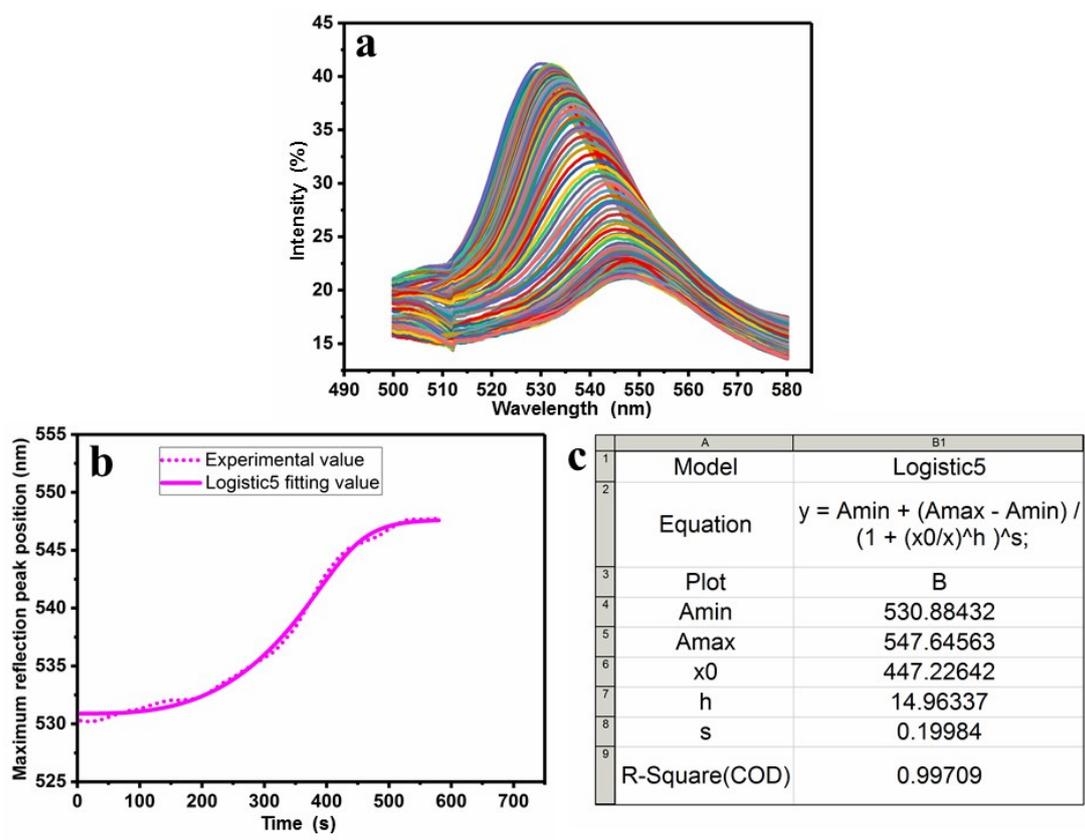
**Figure S11** a) Reflection spectra of PC response to chemical reaction at experiment 9. b) The experimental value and logistic5 fitting value of the corresponding maximum reflection peak position of PC with time including in  $t_{balance}$  and extra 50 s. R-Square is over 0.99.



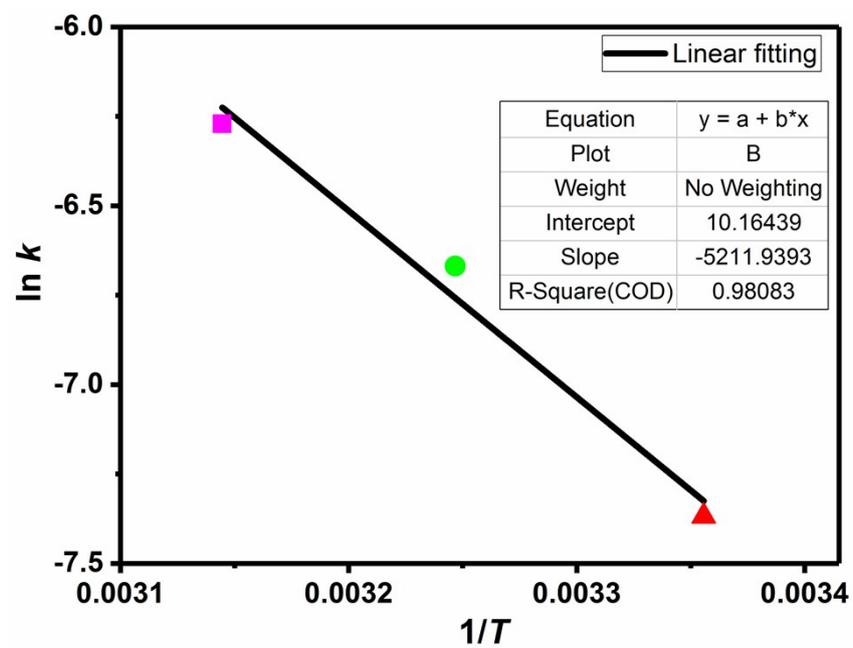
**Figure S12** a) Reflection spectra of PC response to chemical reaction at experiment 10. b) The experimental value and logistic5 fitting value of the corresponding maximum reflection peak position of PC with time including in  $t_{balance}$  and extra 50 s. R-Square is over 0.99.



**Figure S13** a) Reflection spectra of PC response to chemical reaction at experiment 11. b) The experimental value and logistic5 fitting value of the corresponding maximum reflection peak position of PC with time including in  $t_{balance}$  and extra 50 s. R-Square is over 0.99.



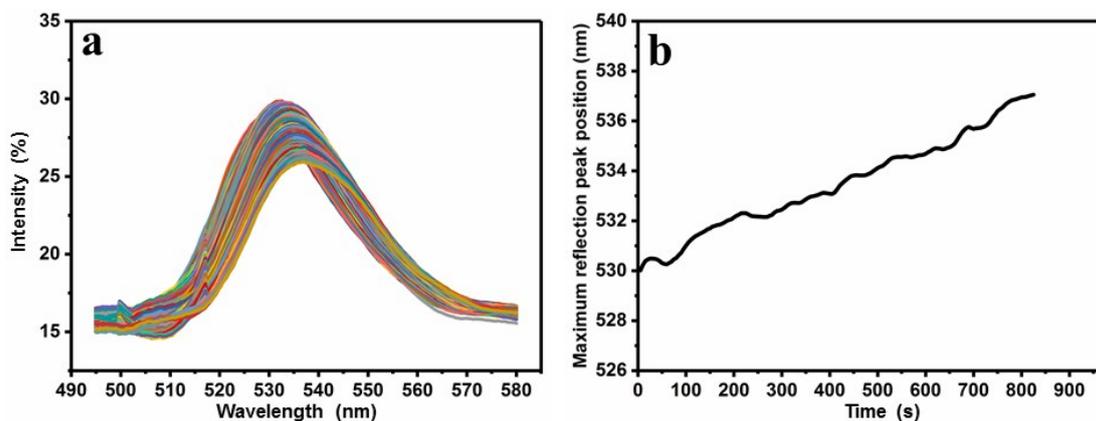
**Figure S14** a) Reflection spectra of PC response to chemical reaction at experiment 12. b) The experimental value and logistic5 fitting value of the corresponding maximum reflection peak position of PC with time including in  $t_{balance}$  and extra 50 s. R-Square is over 0.99.



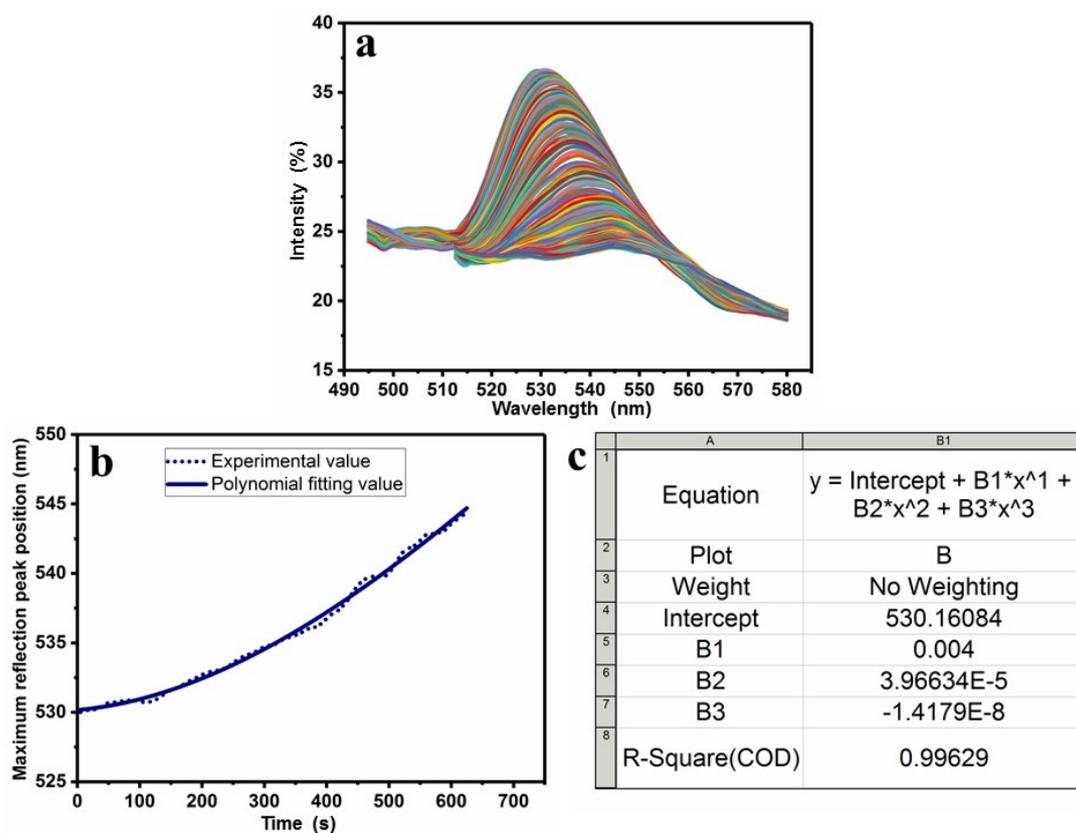
**Figure S15** Relationship of  $\ln k$  and  $1/T$  in 5% of  $\text{AlCl}_3$ . R-Square is over 0.98,  $-E_a/R$  is the slope of -5211.9 J.

**Table S3** The  $t_{\text{balance}}$ , stopband shifts and the average speeds of reflection peak position shift of PC response to chemical reactions under different conditions.  $t_{\text{balance}}$  and  $v'$  present differences under different experimental conditions. B is stand for benzoic acid, S is stand for sulfanilamide, and C is stand for cephalixin.

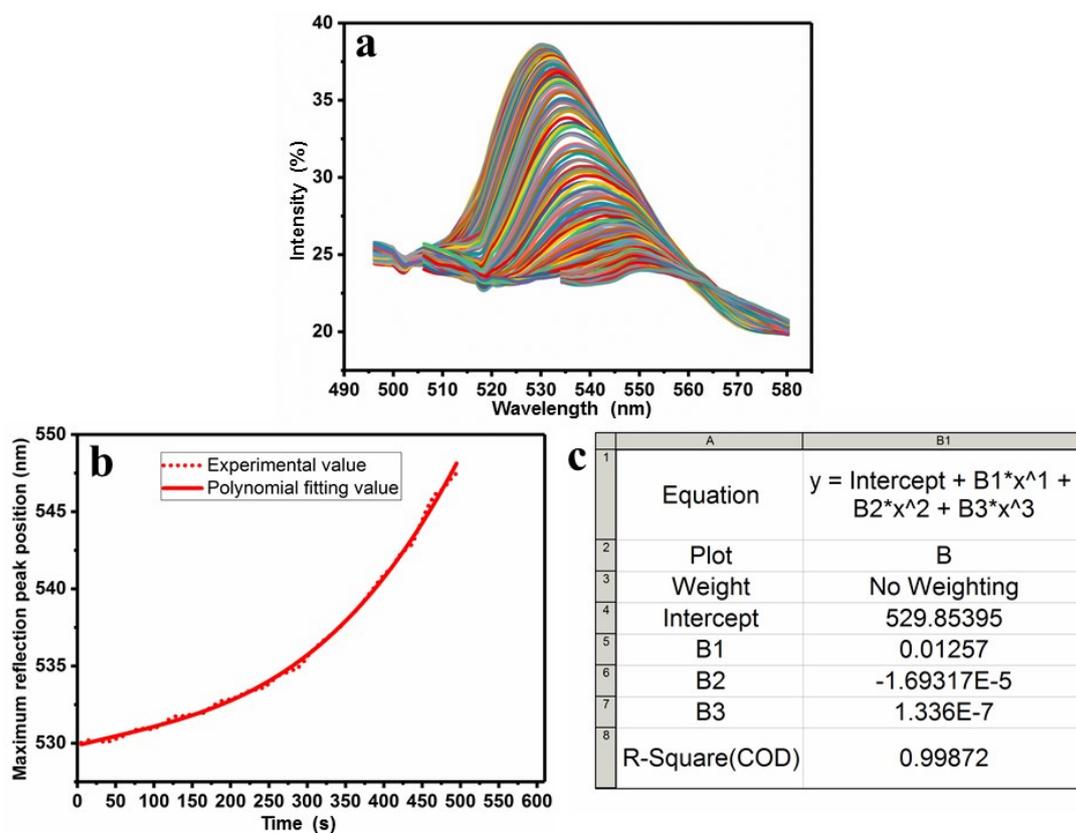
Experim- ental number	Substances	Ratio of H <sub>2</sub> O <sub>2</sub> (%)	Fe <sup>2+</sup> /Fe <sup>3+</sup> (mol/L)	H <sup>+</sup> (mol/L)	$t_{\text{balance}}$ (s)	Stopband shifts (nm)	$v'$ ( $\times 10^{-3}$ nm/s)
13	B-1.0 g/L	-	0.032	-	-	-	-
14	B-1.0 g/L	0.5	0.032	-	625	14.7	23.5
15	B-1.0 g/L	1	0.032	-	495	17.5	35.4
16	B-1.0 g/L	2	0.032	-	505	15.5	30.7
17	B-1.0 g/L	4	0.032	-	260	13.3	51.2
18	B-0.50g/L	1	0.032	-	530	14.1	26.6
19	B-0.25g/L	1	0.032	-	655	17.3	26.4
20	B-1.0 g/L	1	0.016	-	520	16.2	31.2
21	B-1.0 g/L	1	0	-	900	16.3	18.1
22	B-1.0 g/L	1	0.032	0.002	445	12.9	29.0
23	B-1.0 g/L	1	Fe <sup>3+</sup> -0.032	-	600	13.6	22.7
24	S-1.0 g/L	1	0.032	-	520	14.0	26.9
25	S-1.0 g/L	1	0.032	0.0005	530	12.6	23.8
26	S-1.0 g/L	1	0.032	0.002	435	12.7	29.2
27	S-1.0 g/L	1	Fe <sup>3+</sup> -0.032	-	615	15.3	24.9
28	C-1.0 g/L	1	0.032	-	630	11.8	18.7
29	C-1.0 g/L	1	0.032	0.002	530	12.1	22.8
30	C-1.0 g/L	1	Fe <sup>3+</sup> -0.032	-	665	13.2	19.8



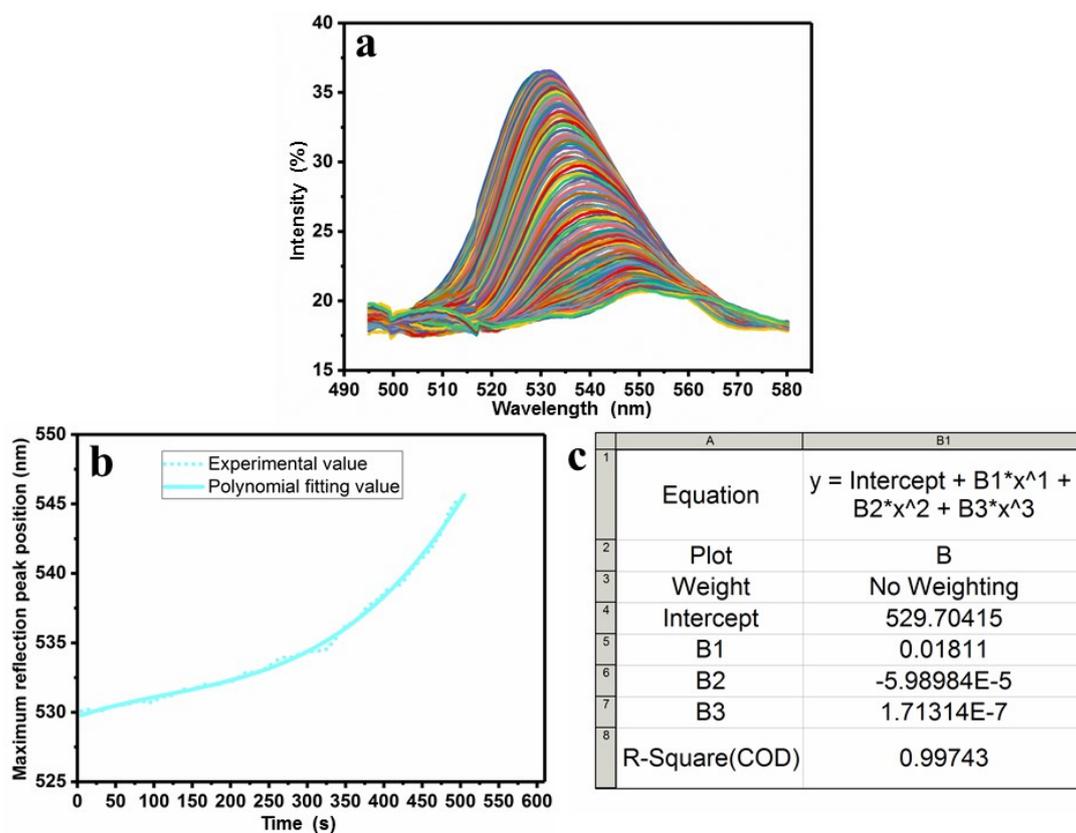
**Figure S16** a) Reflection spectra of PC response to benzoic acid aqueous solution at experiment 13. b) The change curve of the corresponding maximum reflection peak position of PC with time. The stopbands have a little red shift as the solvent volatilizes.



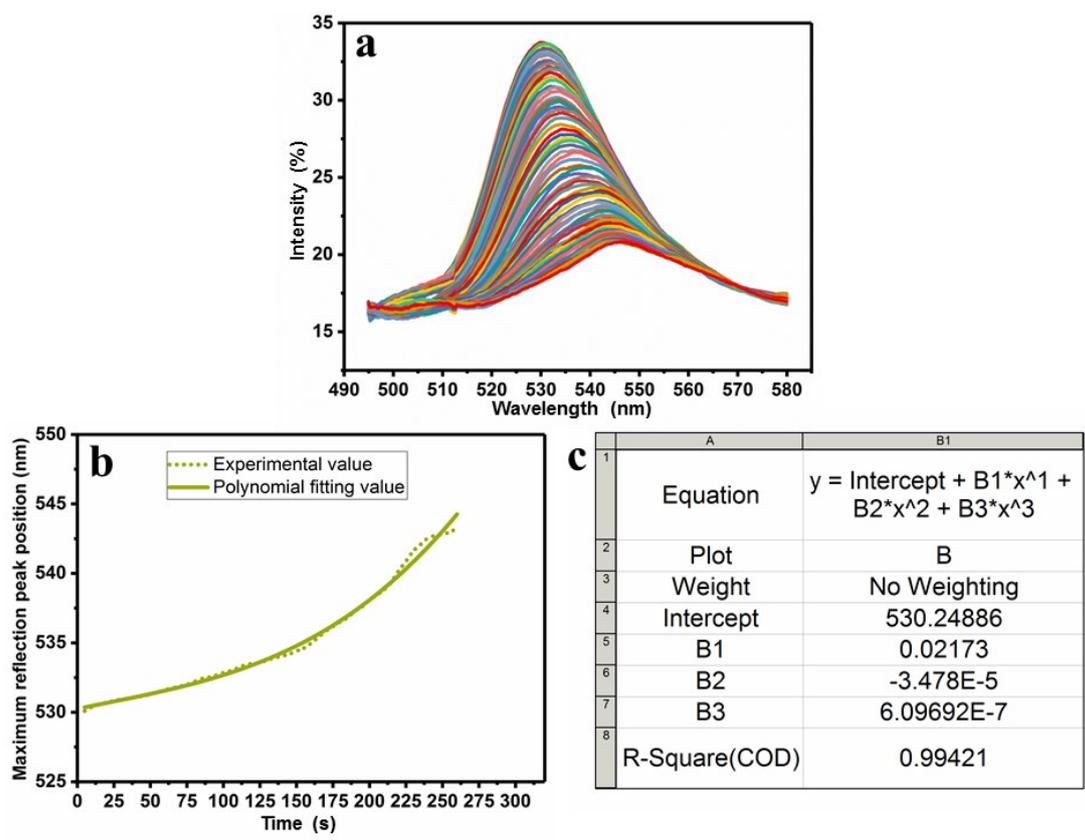
**Figure S17** a) Reflection spectra of PC response to chemical reaction at experiment 14. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99, indicating that the third-order polynomial fitting is reasonable.



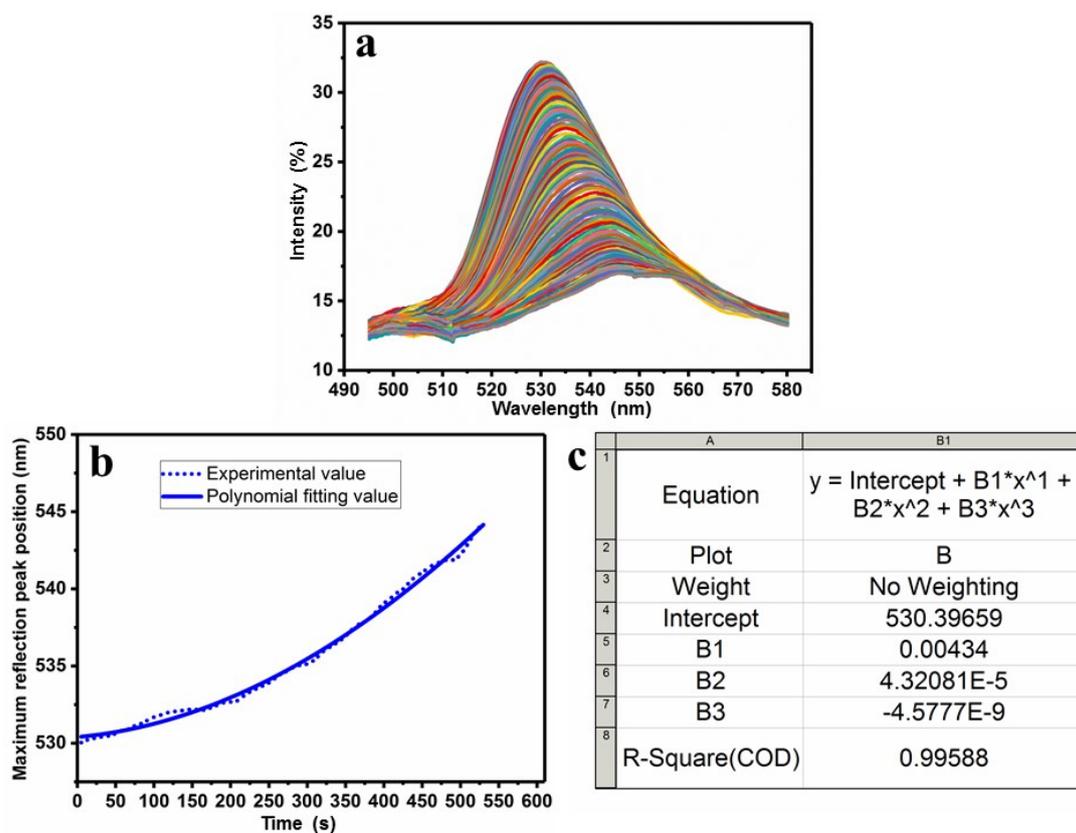
**Figure S18** a) Reflection spectra of PC response to chemical reaction at experiment 15. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



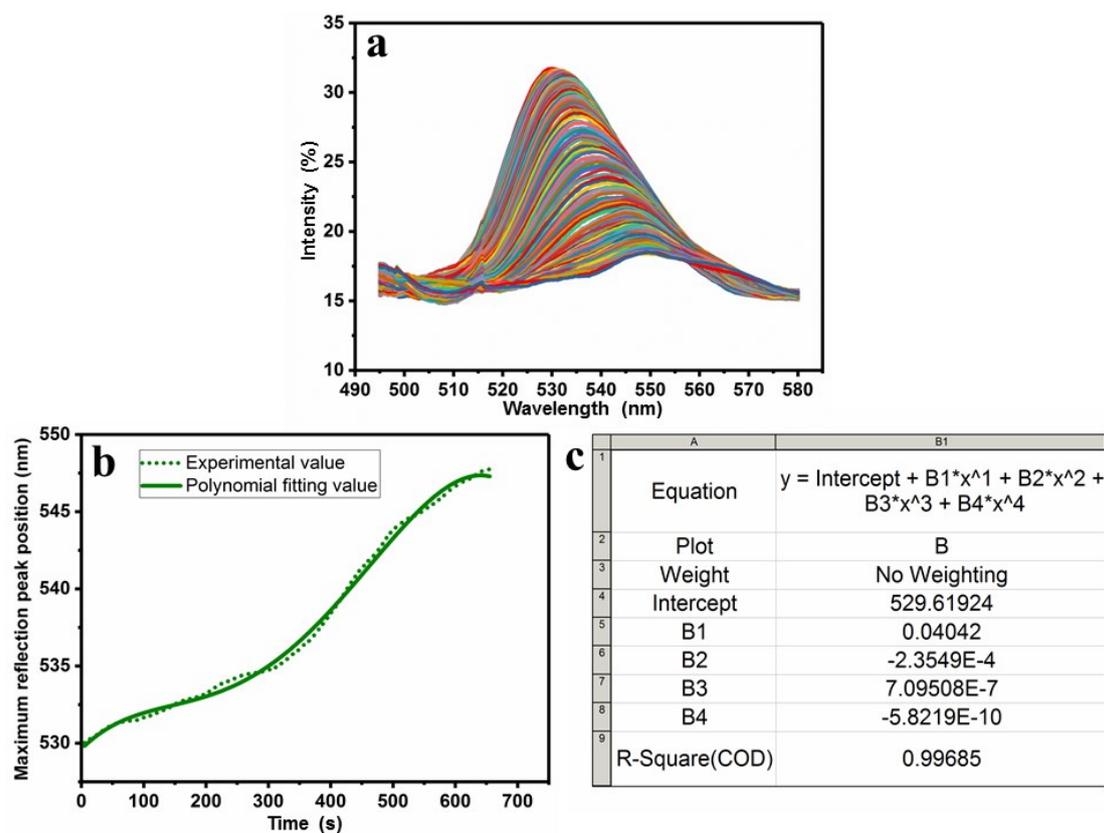
**Figure S19** a) Reflection spectra of PC response to chemical reaction at experiment 16. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



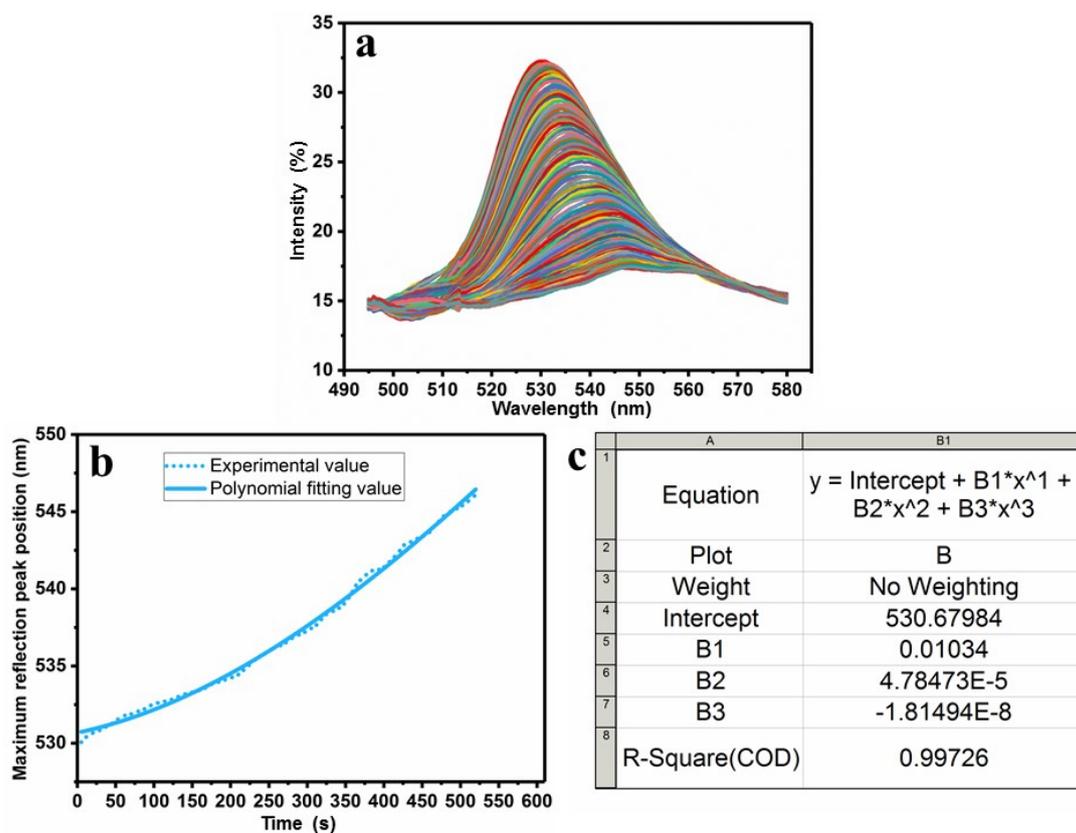
**Figure S20** a) Reflection spectra of PC response to chemical reaction at experiment 17. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



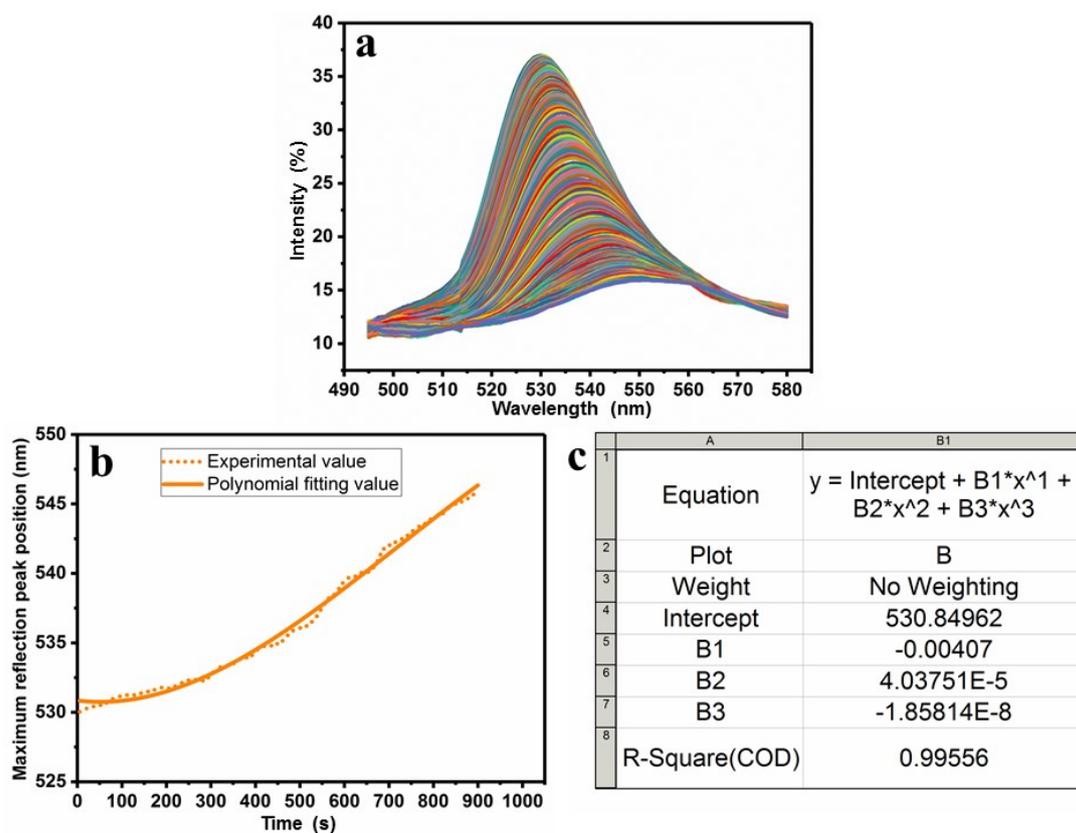
**Figure S21** a) Reflection spectra of PC response to chemical reaction at experiment 18. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



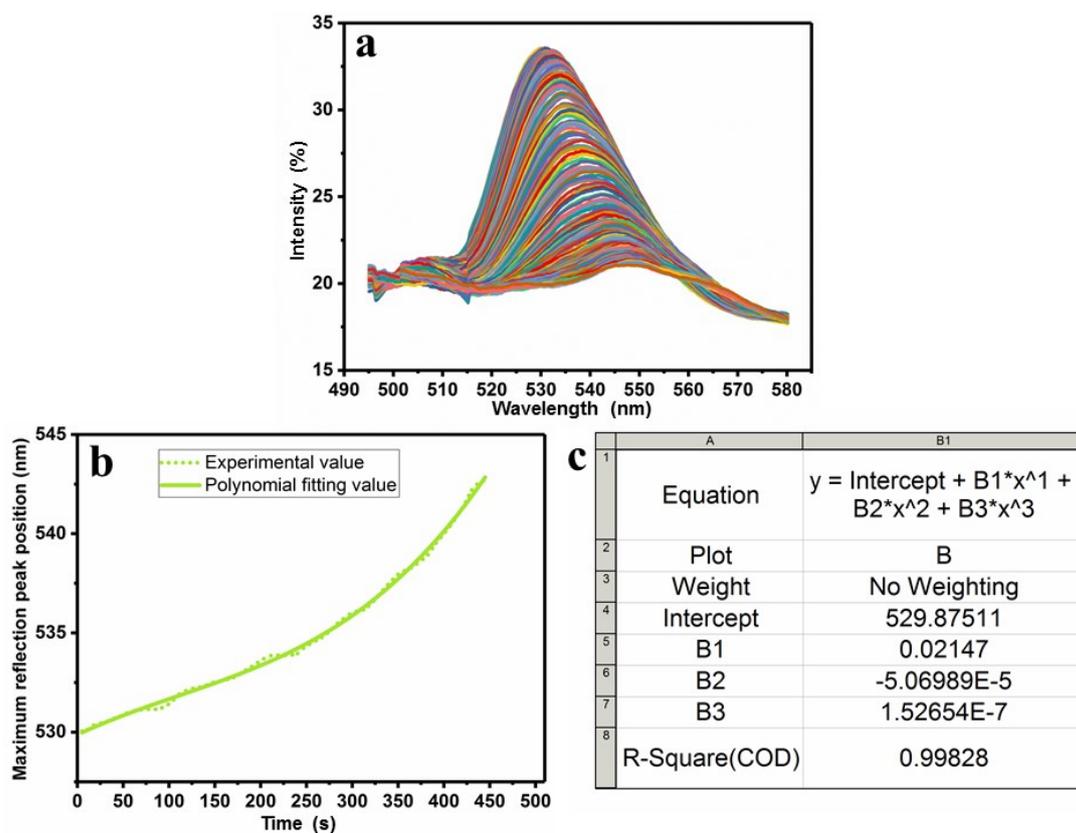
**Figure S22** a) Reflection spectra of PC response to chemical reaction at experiment 19. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99, indicating that the fourth-order polynomial fitting is reasonable.



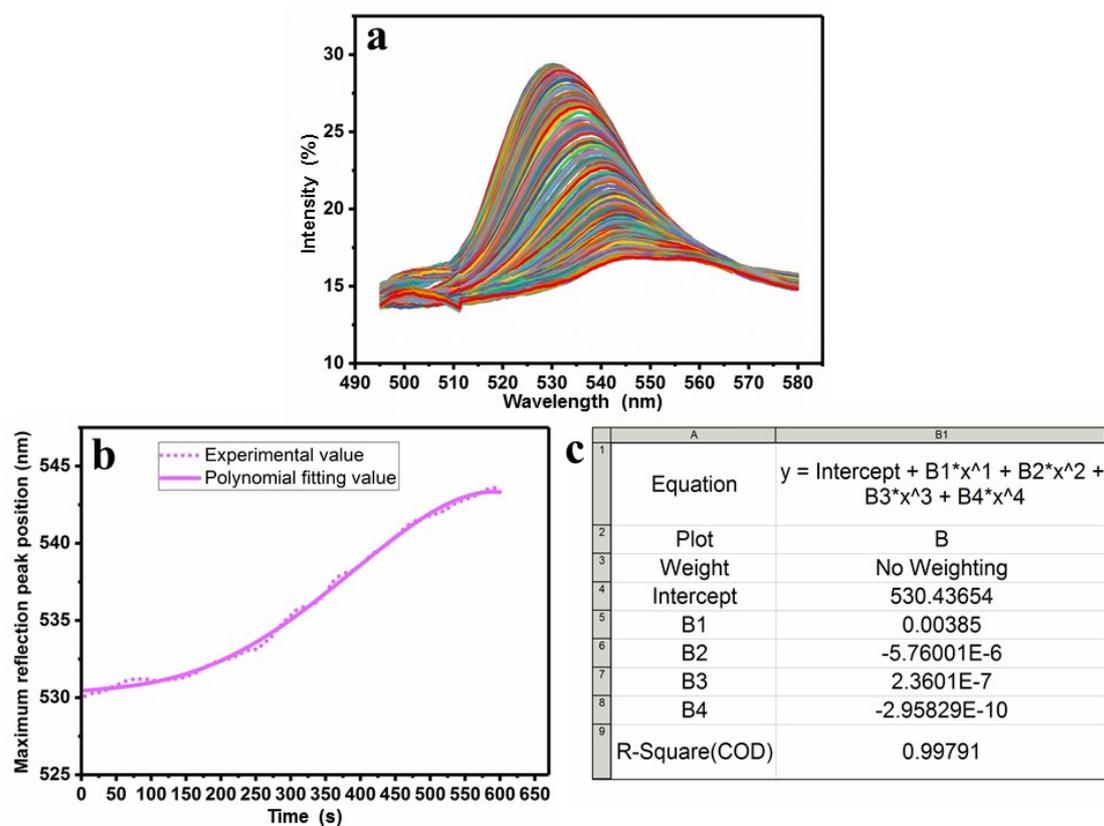
**Figure S23** a) Reflection spectra of PC response to chemical reaction at experiment 20. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



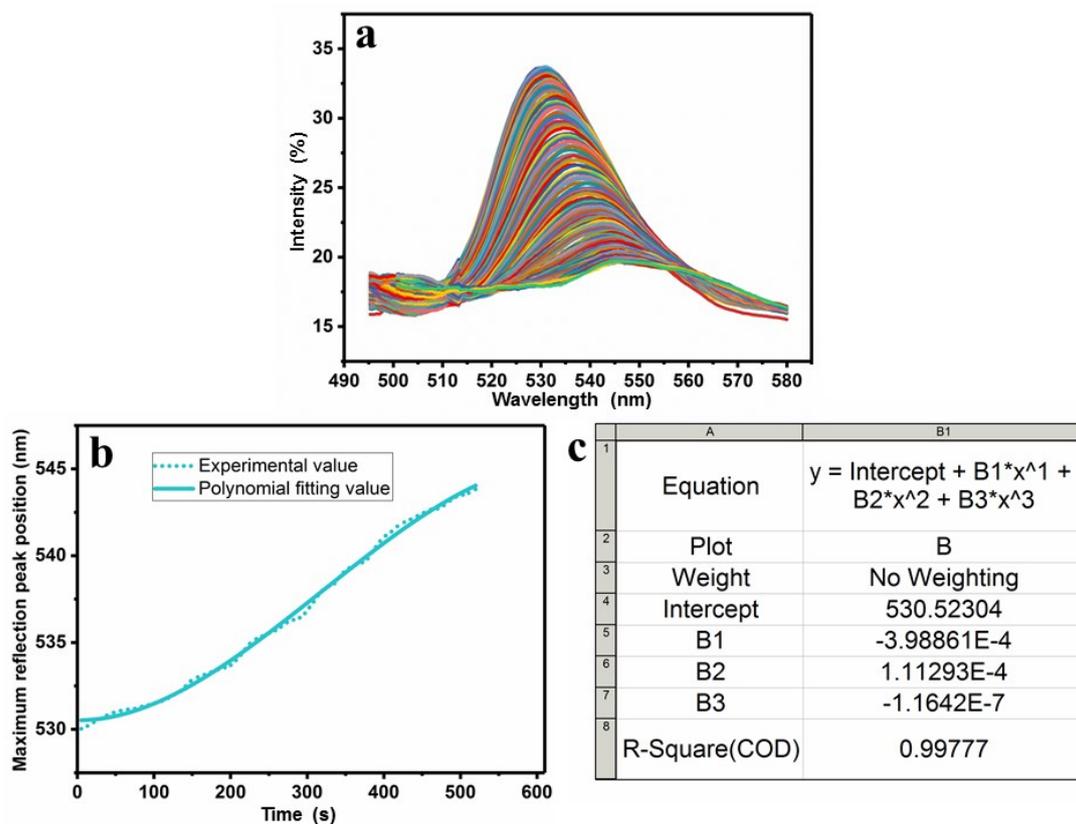
**Figure S24** a) Reflection spectra of PC response to chemical reaction at experiment 21. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



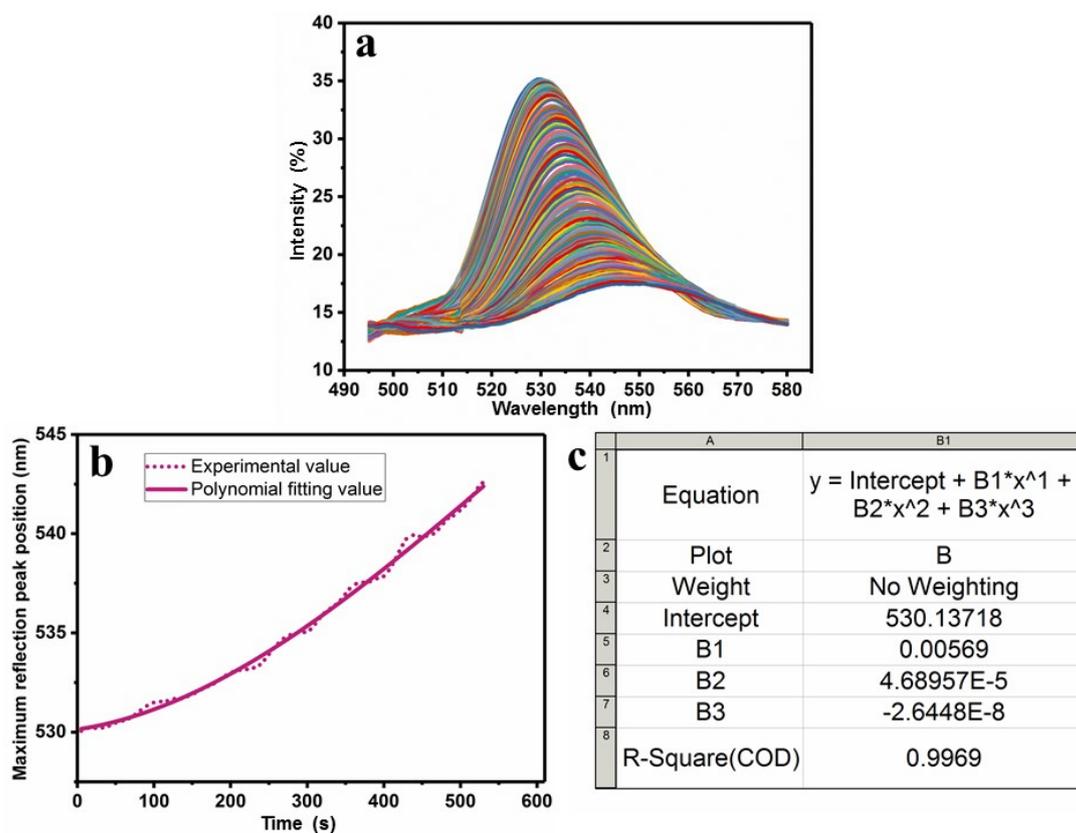
**Figure S25** a) Reflection spectra of PC response to chemical reaction at experiment 22. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



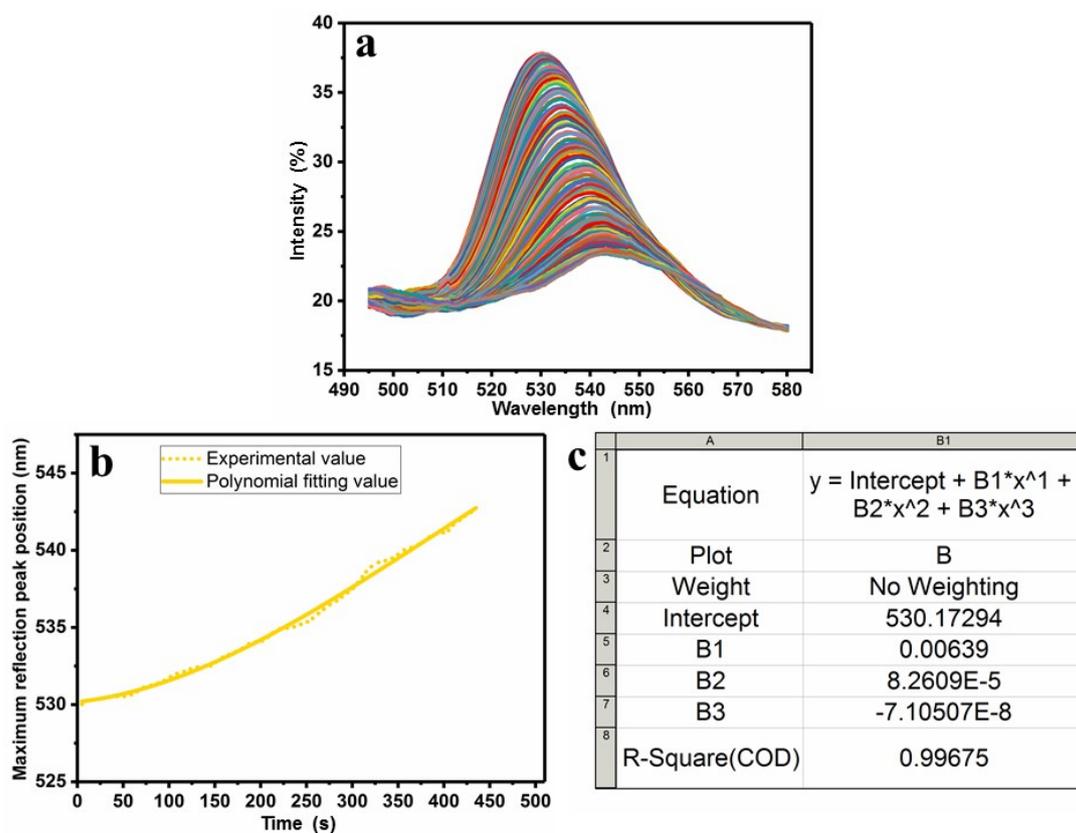
**Figure S26** a) Reflection spectra of PC response to chemical reaction at experiment 23. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99, indicating that the fourth-order polynomial fitting is reasonable.



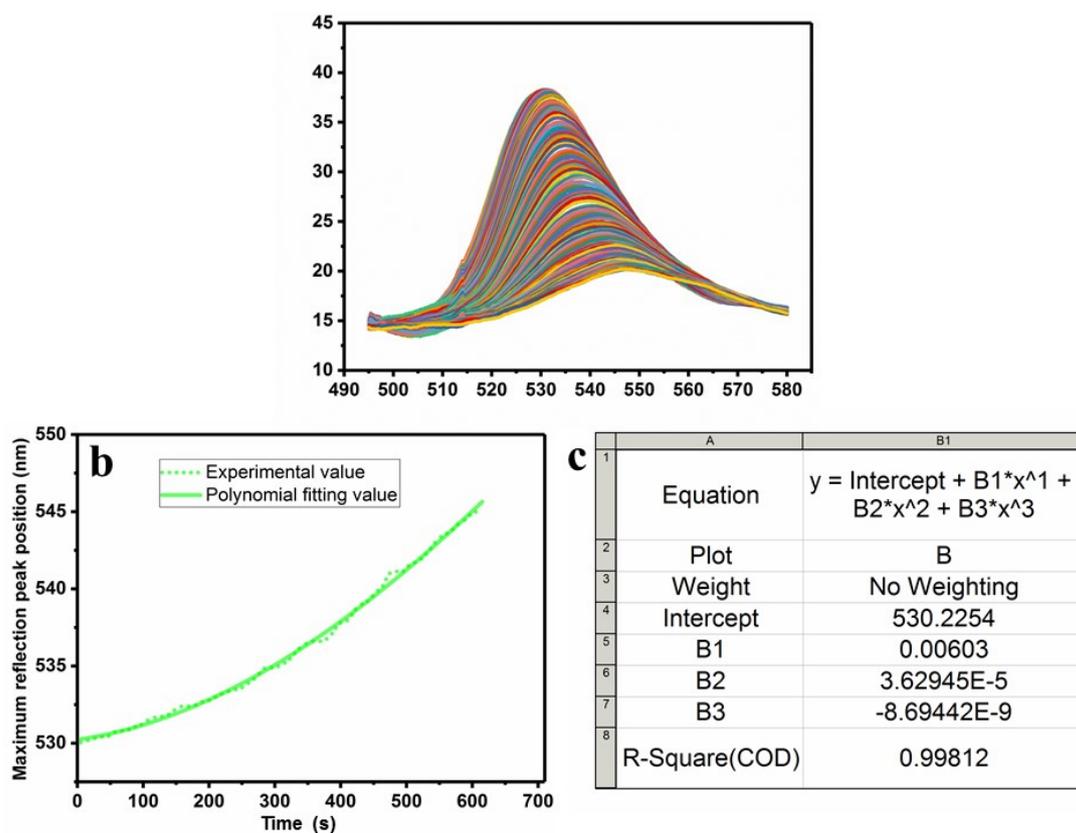
**Figure S27** a) Reflection spectra of PC response to chemical reaction at experiment 24. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



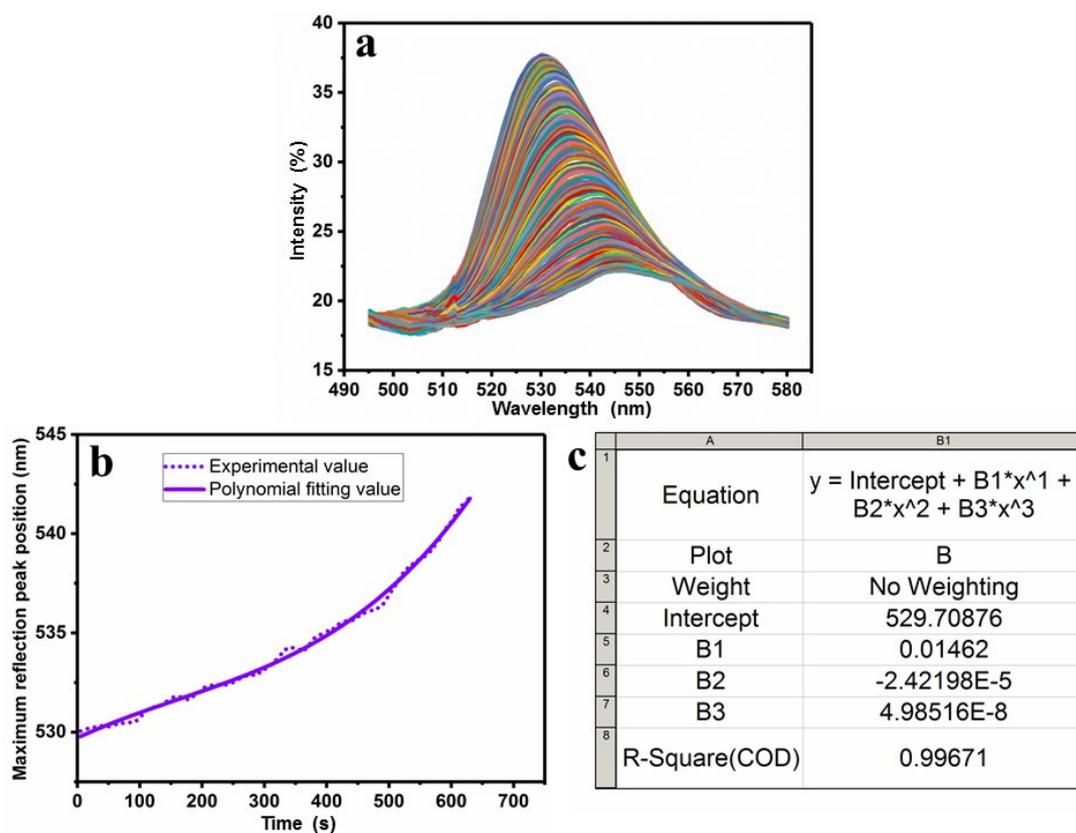
**Figure S28** a) Reflection spectra of PC response to chemical reaction at experiment 25. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



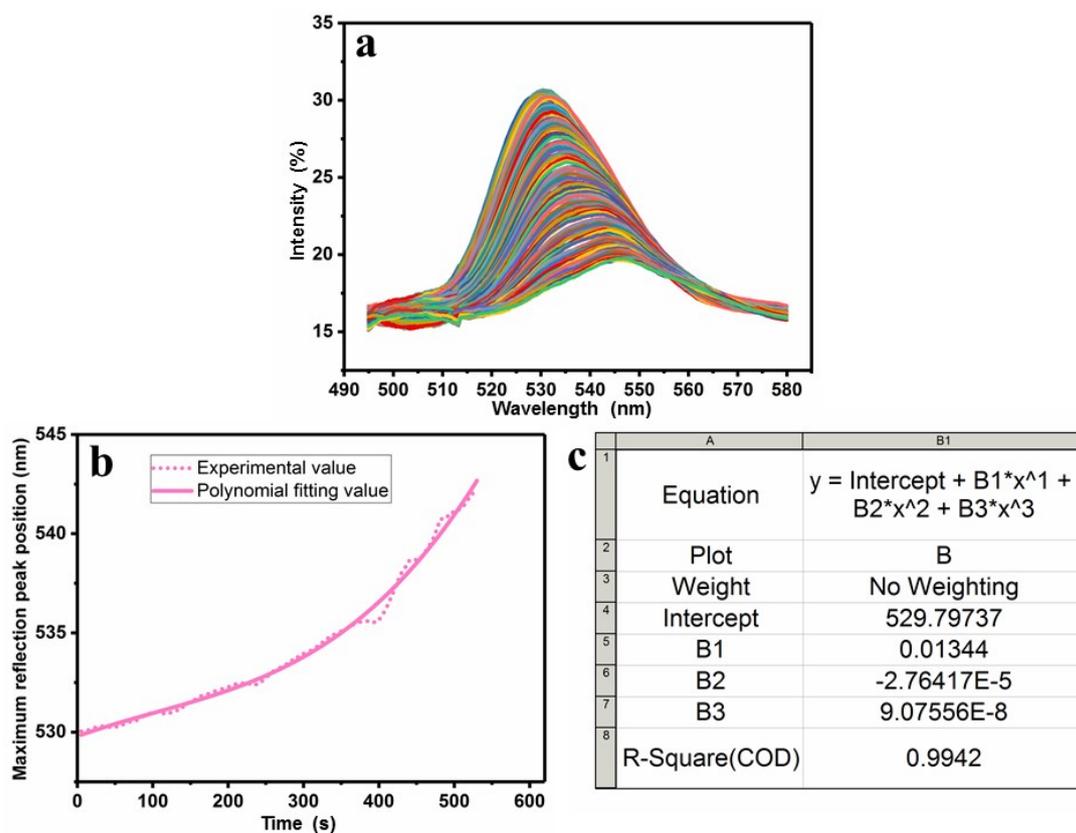
**Figure S29** a) Reflection spectra of PC response to chemical reaction at experiment 26. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



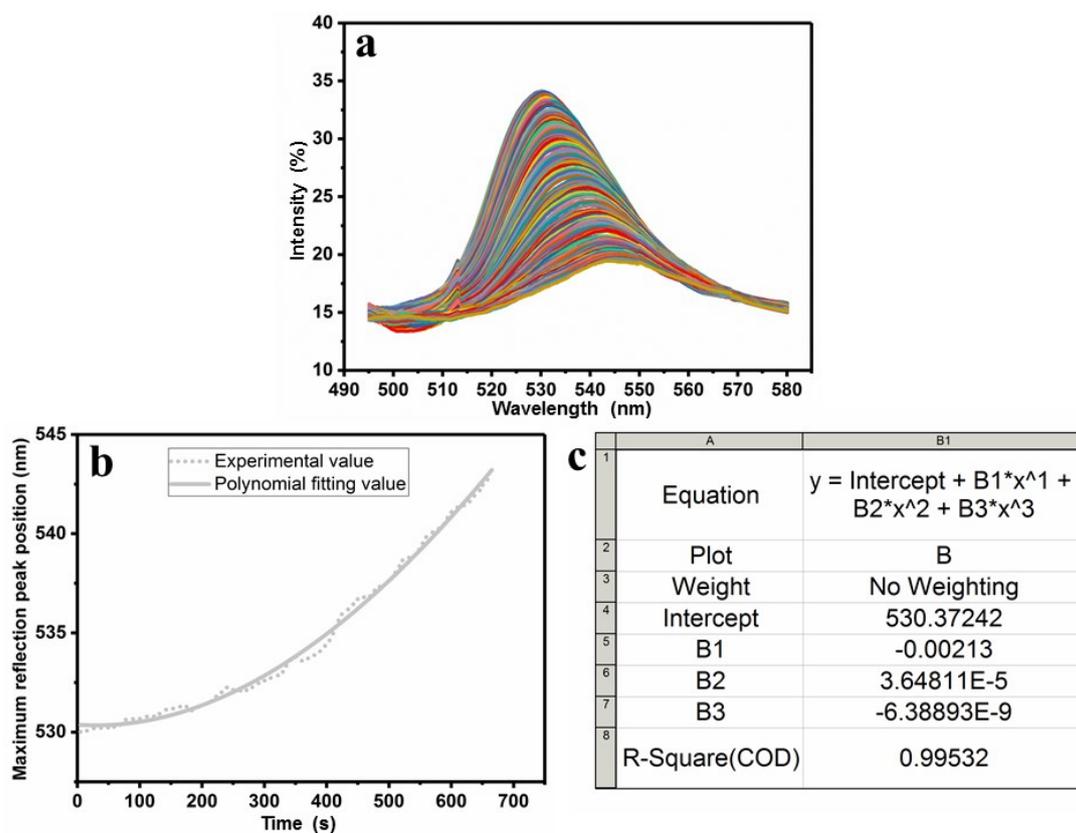
**Figure S30** a) Reflection spectra of PC response to chemical reaction at experiment 27. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



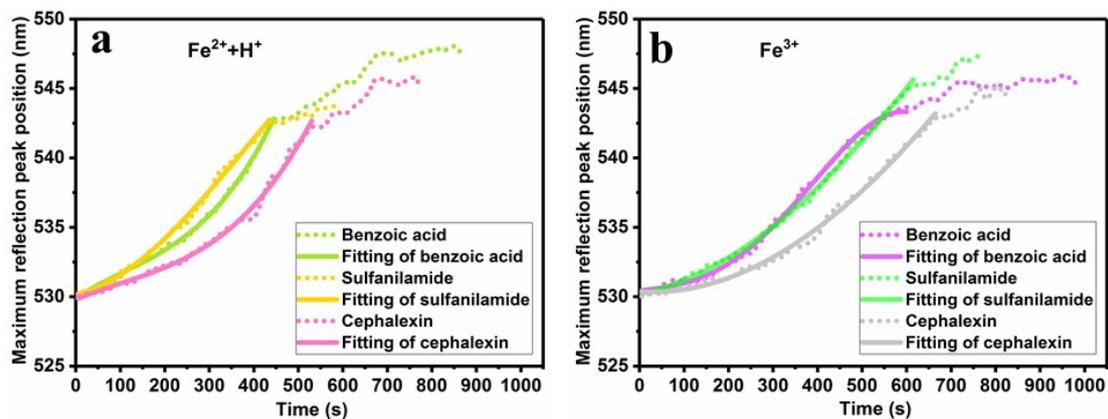
**Figure S31** a) Reflection spectra of PC response to chemical reaction at experiment 28. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



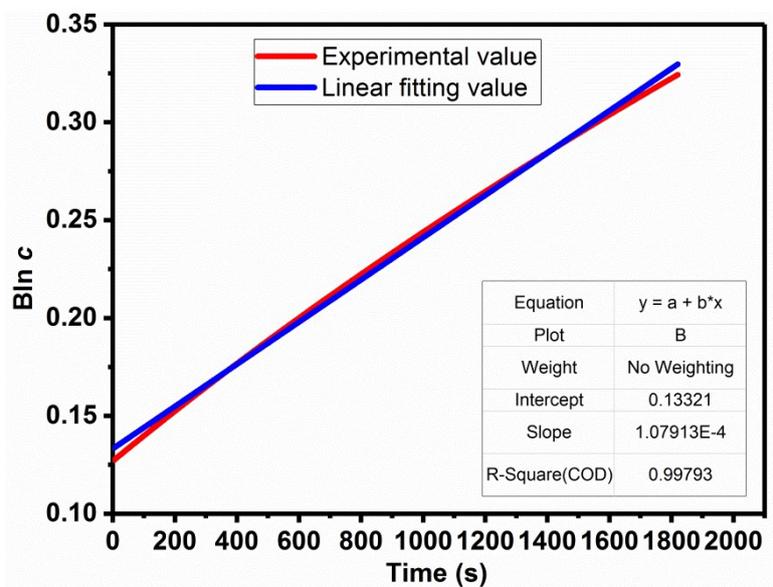
**Figure S32** a) Reflection spectra of PC response to chemical reaction at experiment 29. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



**Figure S33** a) Reflection spectra of PC response to chemical reaction at experiment 30. b) The experimental value and polynomial fitting value of the corresponding maximum reflection peak position of PC with time before  $t_{\text{balance}}$ . R-Square is over 0.99.



**Figure S34** Change curve of the maximum reflection peak positions of PC with time when three chemicals degradation under different chemical conditions: a)  $Fe^{2+}+H^+$  and b)  $Fe^{3+}$ .



**Figure S35** Relationship of  $\ln c$  and  $t$  at experiment 2. R-Square is over 0.99, the relationship is linear.

It offers a detailed course of computing through a simple example.

$$\lambda_t = 2d'n_t \sin \theta \quad (1)$$

$$n_t^2 = 0.74n_s^2 + 0.26n^2 \quad (2)$$

$$\lambda_{t2} = 0.0121t \quad (3)$$

$$\xi = (n - n_{\min}) / (n_{\max} - n_{\min}) \quad (4)$$

$$\frac{dc}{v} = \frac{dn}{dt} \quad (5)$$

$$n-1 = K\rho^{[2]} \quad (6)$$

$$c = B\rho = An \quad (7)$$

$$\frac{dc}{dt} = A \frac{dn}{dt} \quad (8)$$

$$\lambda_t = 2 \times 0.8167 \times d \times n_t = 470 \times 0.8167 \times n_t = 383.85n_t \quad (9)$$

$$n_t^2 = 0.74 \times 1.46 \times 1.46 + 0.26n^2 = 1.5774 + 0.26n^2 \quad (10)$$

$$\lambda_{t2} = 0.0121t \quad (5 \leq t \leq 1820) \quad (11)$$

$$n_{t2} = 3.1523 \times 10^{-5}t \quad (12)$$

$$n^2 = (9.9368 \times 10^{-10}t^2 - 1.5774) / 0.26 \quad (13)$$

$$\lambda_{t2\min} = 530.902 \text{ nm}, \quad n_{\min} = 1.136 \quad (14)$$

$$\lambda_{t2\max} = 552.892 \text{ nm}, \quad n_{\max} = 1.383 \quad (15)$$

### Supporting Reference

[1] C. Xiong, J. Zhao, L. Wang, H. Geng, H. Xu, and Y. Li, *Mater. Horiz.*, 2017, **4**, 862-868.

[2] Slawomir Maj, *Phys Chem Minerals*, 1984, **10**, 133-136.