

Electrodeposited nano-porous and neural network-like Ln@HOF film for SO₂ gas quantitative detection via fluorescent sensing and machine learning

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Electronic supplementary information

Materials and physical measurements

Fig. S1. (a) XPS spectra of Tb 4d electron in Tb@ME-IPA. (b-d) XPS spectra of N 1s electron in ME-IPA, Tb@ME-IPA and **1**. (e-g) XPS spectra of O 1s electron in Tb(NO₃)₃·6H₂O, Tb@ME-IPA and **1**.

Fig. S2. Picture of **1** viewed from different angles.

Fig. S3. (a-d) SEM pictures of **1**.

Fig. S4. (a) SEM image of **1**. (b–e) EDX mapping images of C, N, O and Tb elements in **1**. (f) The element content of C (53.52%), N (36.52%), O (8.39%), Tb (1.57%) elements in EDX energy spectrum of **1**.

Fig. S5. (a) Emission spectrum of ME-IPA upon $\lambda_{\text{ex}} = 310$ nm. (b) Excitation spectrum of **1** by monitoring the 545 nm emission peak. (c) Schematic diagram for TADF-assisted ET and LMCT-induced ET progresses for **1** (ISC: intersystem crossing; RISC: reverse intersystem crossing; TADF: thermally activated delayed fluorescence).

Fig. S6. (a-b) Dependence of emission intensity for **1** on temperature (30–60 °C) upon $\lambda_{\text{ex}} = 290$ nm.

Fig. S7. Emission spectra of **1** taken out from different gas atmospheres with a concentration of 10⁻² mol/L ($\lambda_{\text{ex}} = 290$ nm).

Fig. S8. (a) Emission spectra of **1** and 1-SO₂ ($\lambda_{\text{ex}} = 290$ nm). (b) CIE diagram for indicating the emitting color transfer of **1** from (0.2103, 0.7623) to (0.1673, 0.0452) ($\lambda_{\text{ex}} = 290$ nm).

Fig. S9. (a) Response time of **1** toward SO₂. (b) Luminescence intensity of 545 nm peak for **1** after seven repetitions in recycling experiment of SO₂ sensing.

Fig. S10. (a) SEM image of 1-SO₂. (b–f) EDX mapping images of C, N, O and Tb elements in 1-SO₂. (g) The element content of C (45.71%), N (35.97%), O (16.36%), S (0.32%) and Tb (1.64%) elements in EDX energy spectrum of 1-SO₂.

Fig. S11. (a) Emission spectrum of 1-SO₂ ($C_{\text{SO}_2} = 10^{-2}$ M). (b) Decay lifetime of 545 nm emission peak of **1** ($\lambda_{\text{ex}} = 290$ nm). (c) Emission spectra of ME and IPA powders. (d) PXRD patterns of **1** and 1-SO₂.

Fig. S12. (a) Emission spectra of Tb@ME-IPA in various anion solution ($C = 10^{-2}$ M) ($\lambda_{\text{ex}} = 290$ nm). (b) Emission intensity of 545nm peak in various anion solution ($C = 10^{-2}$ M). (c) Emission spectra of Tb@ME-IPA and Tb@ME-IPA-SO₃²⁻ ($C = 10^{-2}$ M) ($\lambda_{\text{ex}} = 290$ nm). (d) Decay lifetimes of 545 nm emission peak for Tb@ME-IPA and Tb@ME-IPA-SO₃²⁻ ($C = 10^{-2}$ M) ($\lambda_{\text{ex}} = 290$ nm).

Fig. S13. (a) Emission spectra of Tb@ME-IPA in various SO₃²⁻ solutions with a successive concentration ($C = 10^{-8}$ – 10^{-2} M) ($\lambda_{\text{ex}} = 290$ nm). (b) Dependence of emission intensity of 545 and 380 nm peaks on SO₃²⁻ concentration. (c) Emitting pictures of Tb@ME-IPA in various SO₃²⁻ solutions with a successive

concentration ($C = 10^{-8}$ - 10^{-2} M) ($\lambda_{ex} = 290$ nm). (d) Dependence of emission intensity ratio of 380 and 545 nm peaks on SO_3^{2-} concentration ($C = 10^{-8}$ - 10^{-2} M) (e) Calibration curves of Tb@ME-IPA toward SO_3^{2-} in the concentration range of 10^{-8} - 10^{-2} M. (f) Response time of Tb@ME-IPA toward SO_3^{2-} .

Fig. S14. (a) Emission spectra of Tb@ME-IPA in various serum components ($C = 10^{-2}$ M) ($\lambda_{ex} = 290$ nm). (b) Histogram of 545 nm emission peak of Tb@ME-IPA in various serum components ($C = 10^{-2}$ M). (c) Emission spectra of Tb@ME-IPA in serum system in various SO_3^{2-} solutions with a successive concentration ($C = 10^{-8}$ - 10^{-2} M) ($\lambda_{ex} = 290$ nm). (d) Dependence of emission intensity of 545 and 380 nm peaks on SO_3^{2-} concentration. (e) Dependence of emission intensity ratio of 380 and 545 nm peaks on SO_3^{2-} concentration (10^{-7} - 10^{-2} M). (f) Calibration curves of Tb@ME-IPA toward SO_3^{2-} in the concentration range of 10^{-7} - 10^{-2} M.

Fig. S15. Network training curve of the BPNN.

Fig. S16. Deviation curve of the BPNN (OV: original value; CV: calculated value).

Table S1. The reaction equations for preparation of various gases.

Table S2. Element contents of C, N, O, Tb in EDX energy spectrum **1** and C, N, O, S, Tb in EDX energy spectrum **1-SO₂**.

Table S3. Summary of decay lifetime of **1**, **1-SO₂**, Tb@ME-IPA, and Tb@ME-IPA- SO_3^{2-} .

Table S4. Summary of emission transitions and experimental energy gaps of ME-IPA and Tb^{3+} ions.

Table S5. Summary of R.G.B. of emitting color of **1** exposed in various SO_2 concentration (10^{-6} - 10^{-2} M).

Table S6. Summary of input and output information during the training of BPNN for SO_2 detection.

Table S7. Network structure information.

Table S8. The summary of mean square error (MSE), original value (OV), calculated value (CV), variance (Var.)

Table S9. The summary of input and output information in real batch calculation during the test of BPNN.

Table S10. The matlab code of this BPNN.

Materials and physical measurements

All reagents were used without further purification. Powder X-ray diffraction (PXRD) patterns were collected with a Bruker D8 ADVANCE diffractometer using Cu $K\alpha$ radiation at 40 mA and 40 kV. SEM was performed on a Hitachi S-4800 field emission scanning electron microscope operating at 3 kV. Energy dispersive X-ray spectroscopy (EDX) and the EDX mapping image were obtained by the scanning electron microscope operating at 15 kV. X-ray photoelectron (XPS) spectra were recorded under ultrahigh vacuum ($<10^{-6}$ Pa) at a pass energy of 93.90 eV with an Axis Ultra DLD spectrometer (Kratos) by using a Mg $K\alpha$ (1253.6 eV) anode. All binding energies were adjusted by using contaminant carbon (C 1s = 284.8 eV). Fourier transform infrared (FT-IR) spectra were recorded using a Nicolet IS10 infrared spectrophotometer. The photoluminescence (PL) spectra, kinetics scan curve and phosphorescence decay lifetime curve were recorded on an Edinburgh FLS920 spectrophotometer with a 450 W xenon lamp as an excitation source.

The HOMO–LUMO energy levels were calculated by the DFT method at the b3lyp/6-31g level in the Gaussian 09W program package.

The BPNN model was constructed in Maishi Neural Network program package.

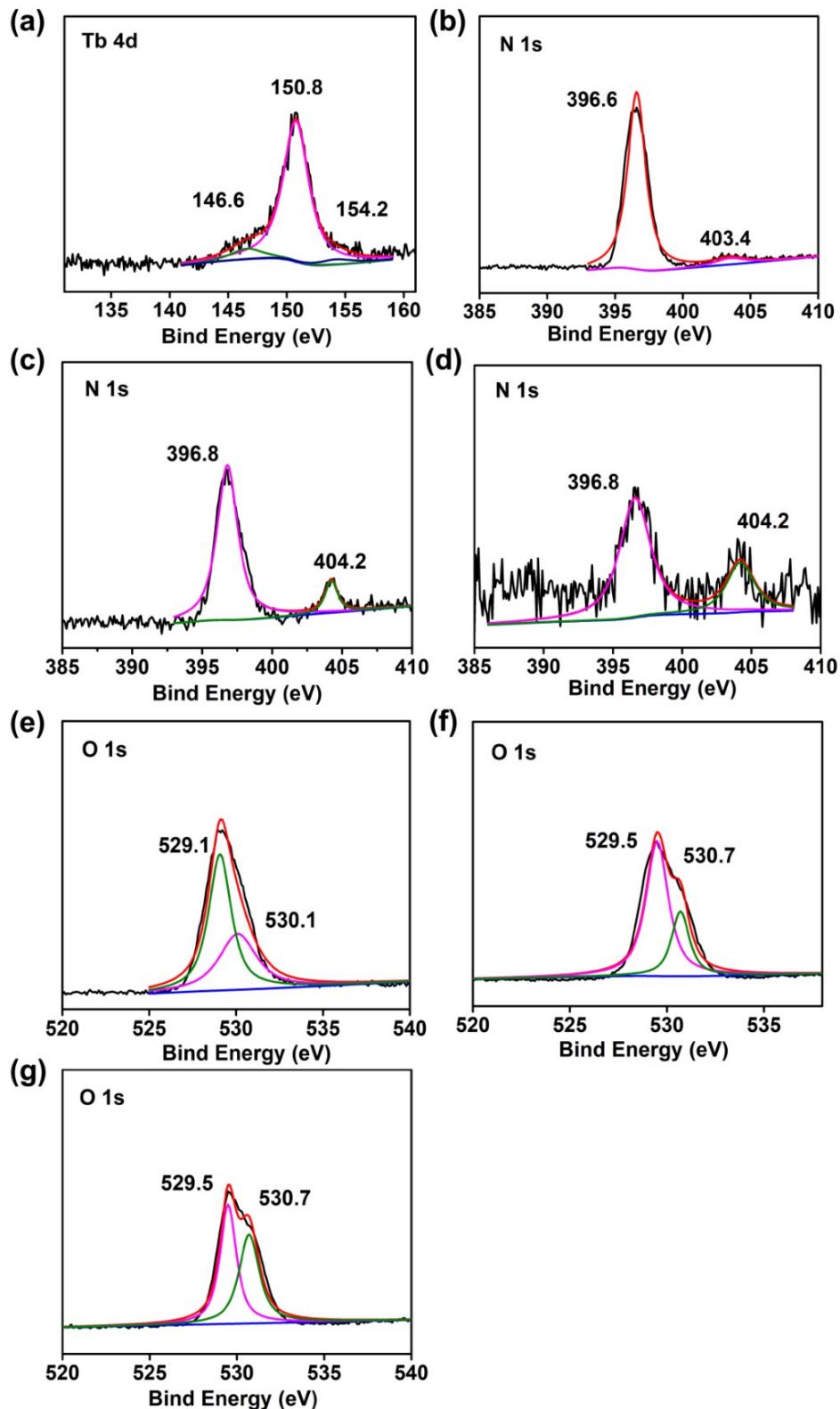


Fig. S1. (a) XPS spectra of Tb 4d electron in Tb@ME-IPA. (b-d) XPS spectra of N 1s electron in ME-IPA, Tb@ME-IPA and **1**. (e-g) XPS spectra of O 1s electron in $\text{Tb}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$, Tb@ME-IPA and **1**.

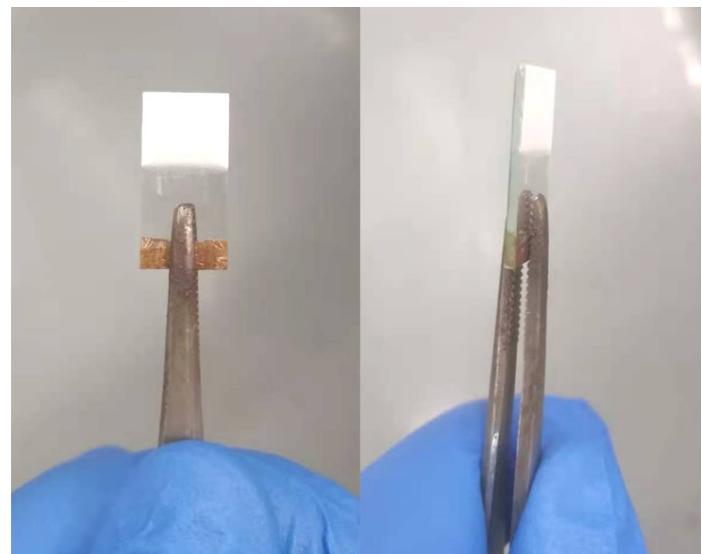


Fig. S2. Picture of **1** viewed from different angles.

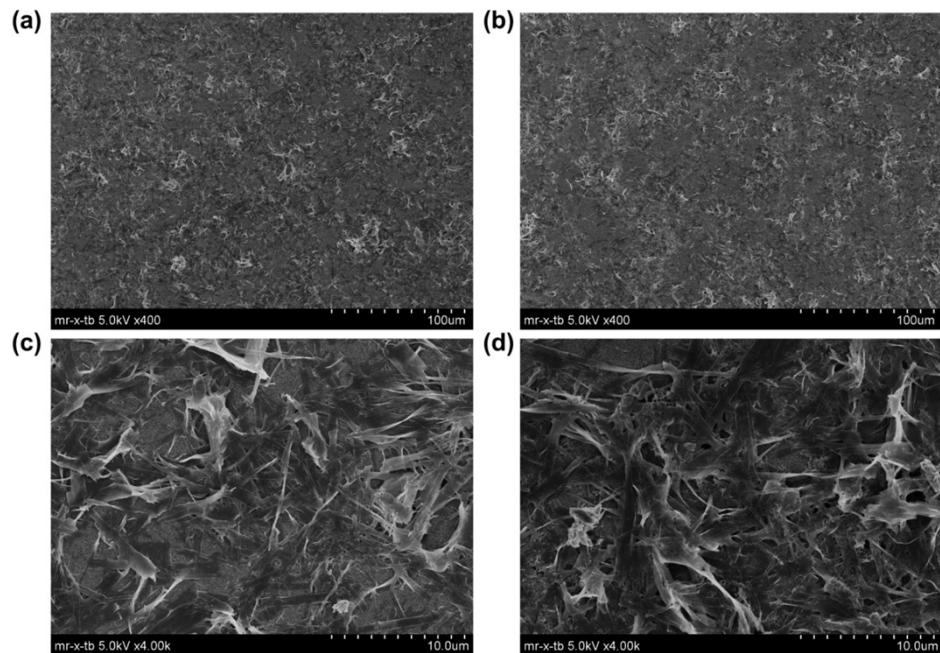


Fig. S3. (a-d) SEM pictures of **1**.

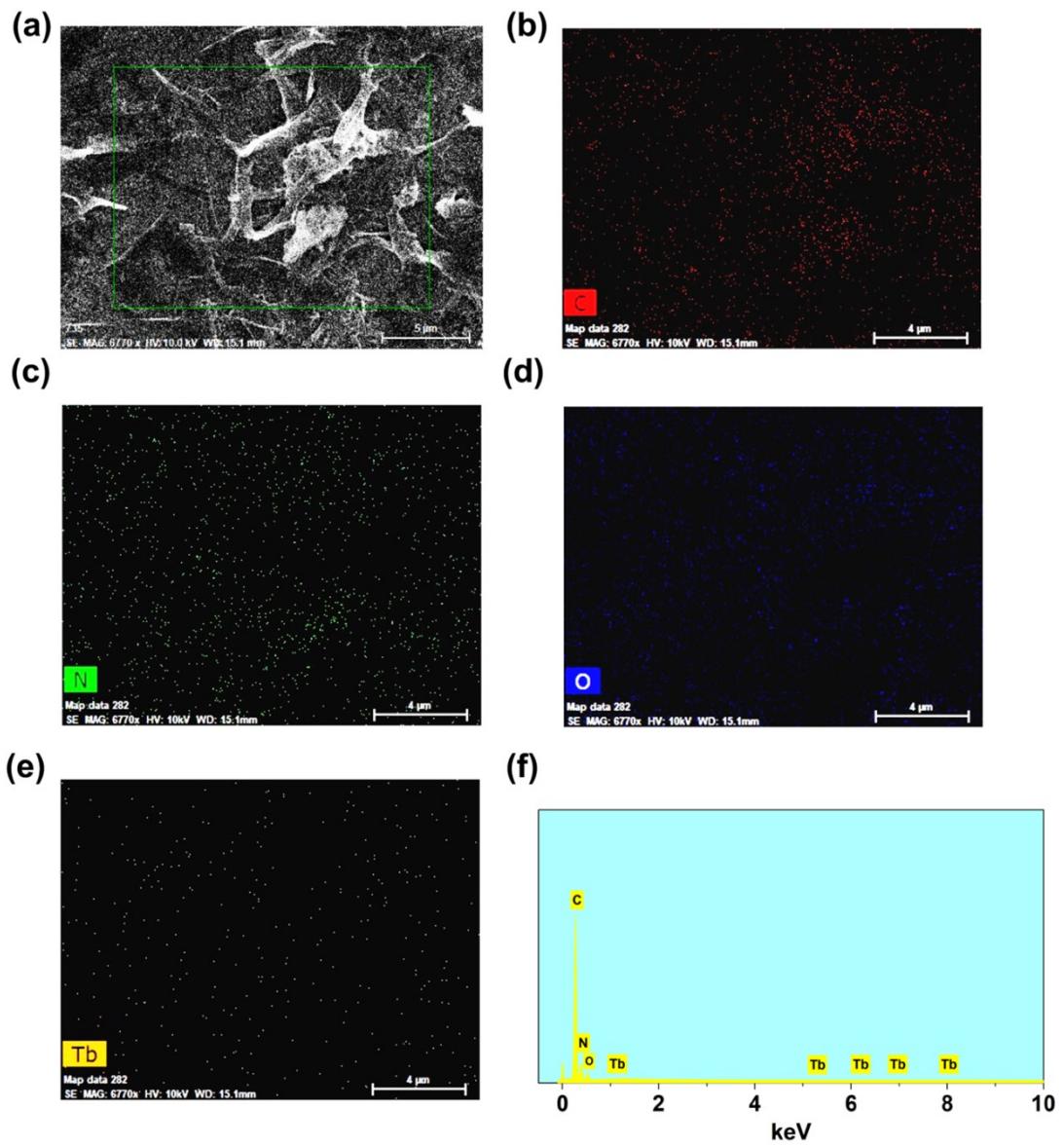


Fig. S4. (a) SEM image of **1**. (b–e) EDX mapping images of C, N, O and Tb elements in **1**. (f) The element content of C (53.52%), N (36.52%), O (8.39%), Tb (1.57%) elements in EDX energy spectrum of **1**.

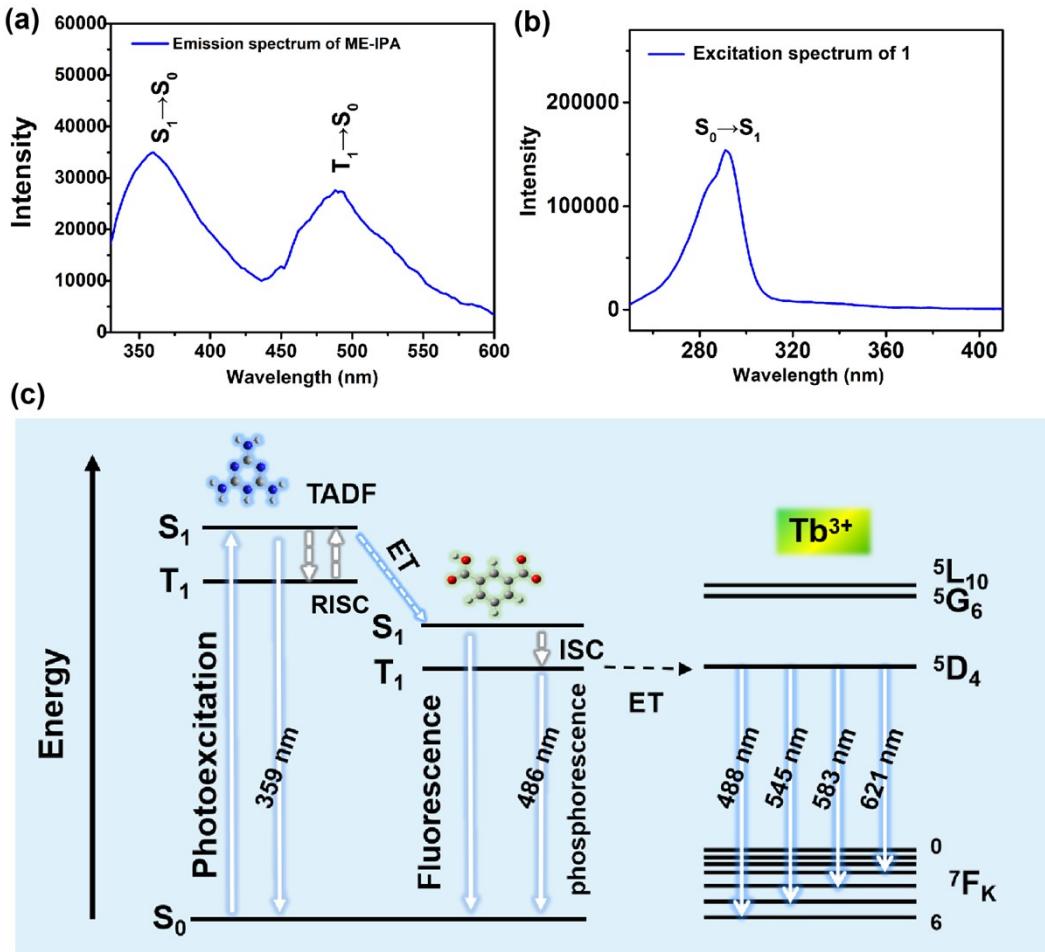


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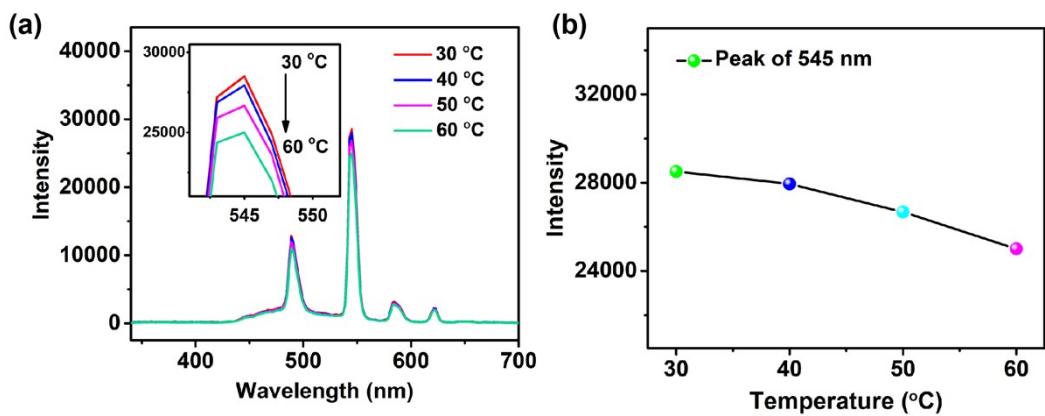


Fig. S6. (a-b) Dependence of emission intensity for **1** on temperature (30–60 °C) upon $\lambda_{\text{ex}} = 290$ nm.

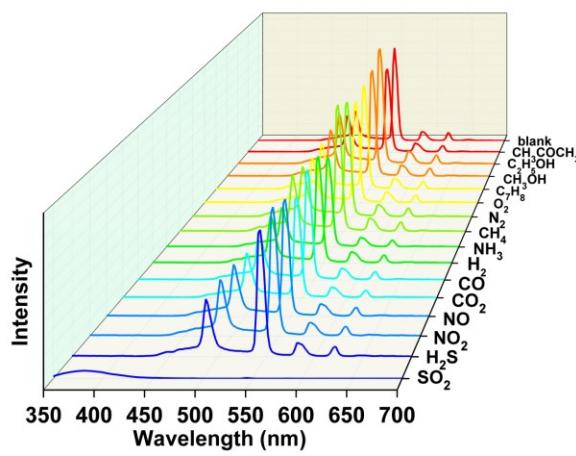


Fig. S7. Emission spectra of **1** taken out from different gas atmospheres with a concentration of 10^{-2} mol/L ($\lambda_{\text{ex}} = 290$ nm).

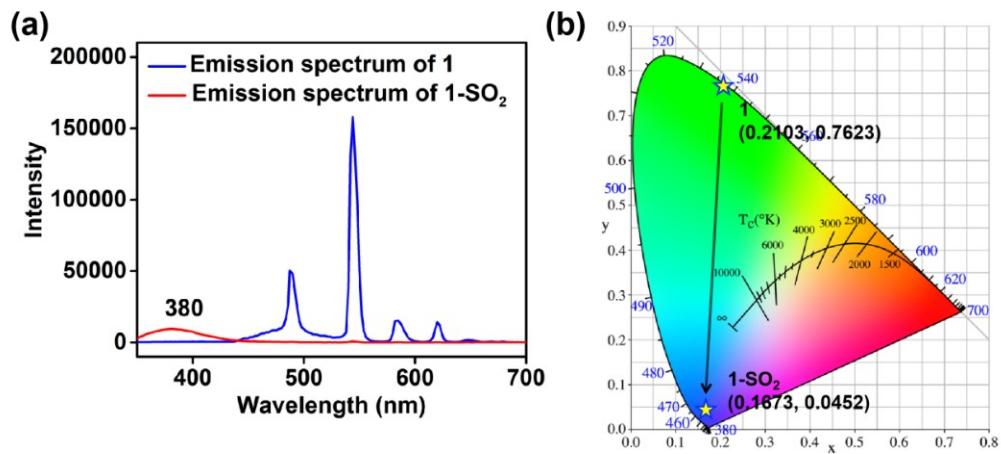


Fig. S8. (a) Emission spectra of **1** and **1**-SO₂ ($\lambda_{\text{ex}} = 290$ nm). (b) CIE diagram for indicating the emitting color transfer of **1** from (0.2103, 0.7623) to (0.1673, 0.0452) ($\lambda_{\text{ex}} = 290$ nm).

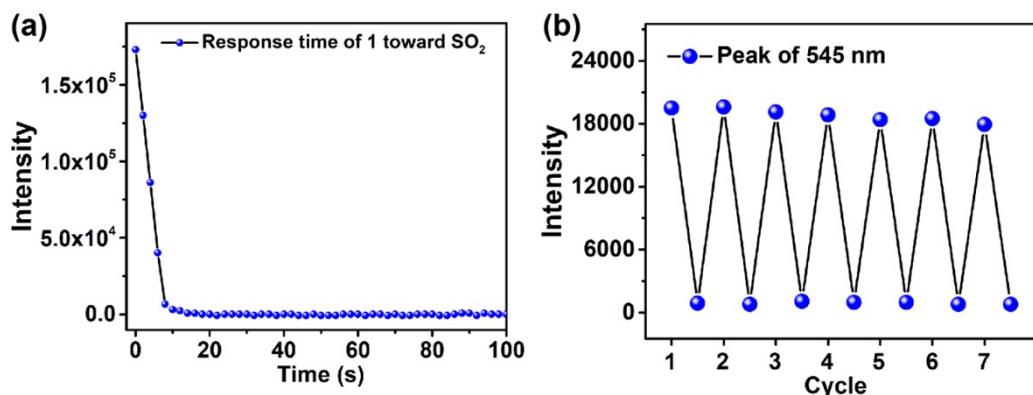


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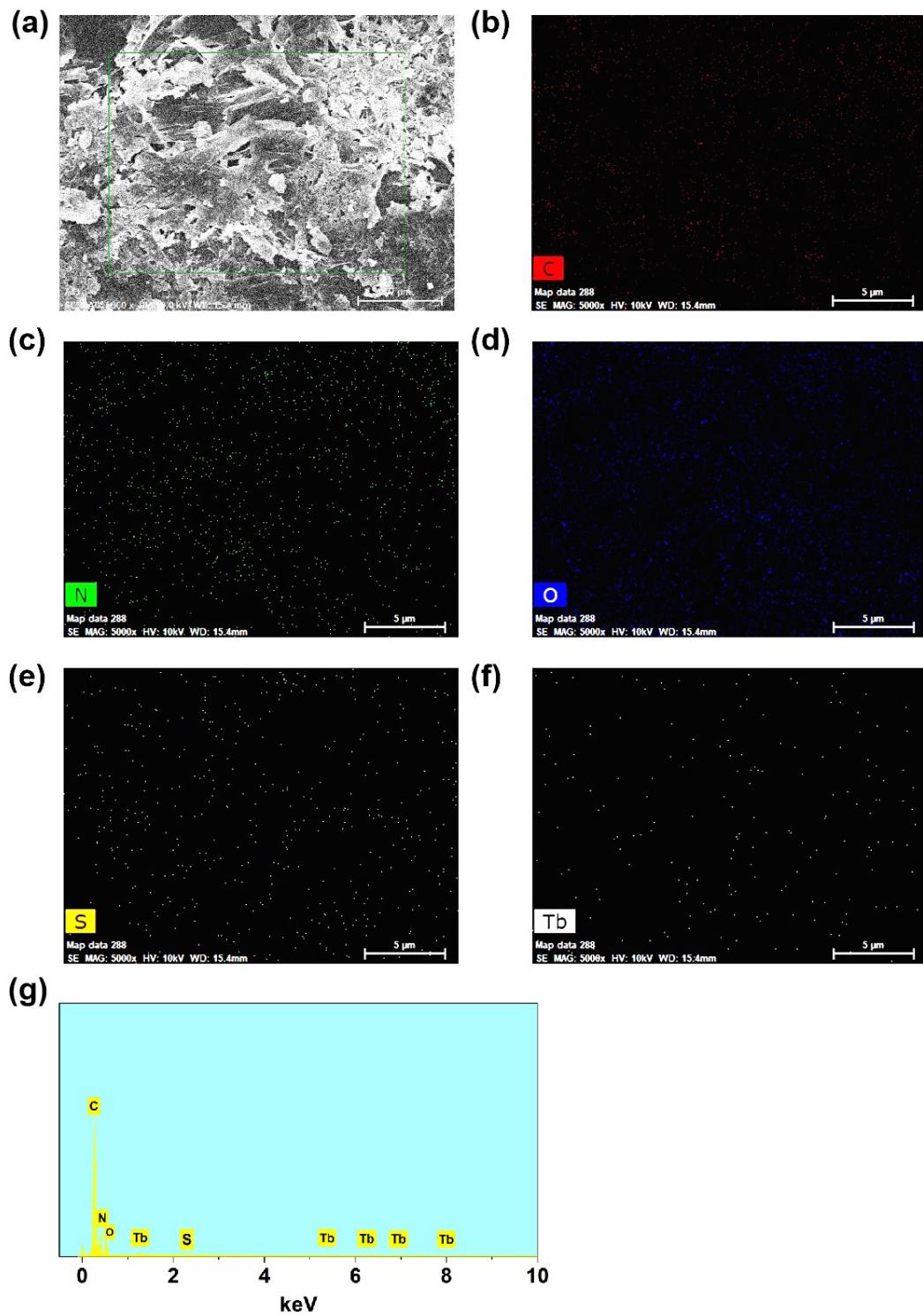


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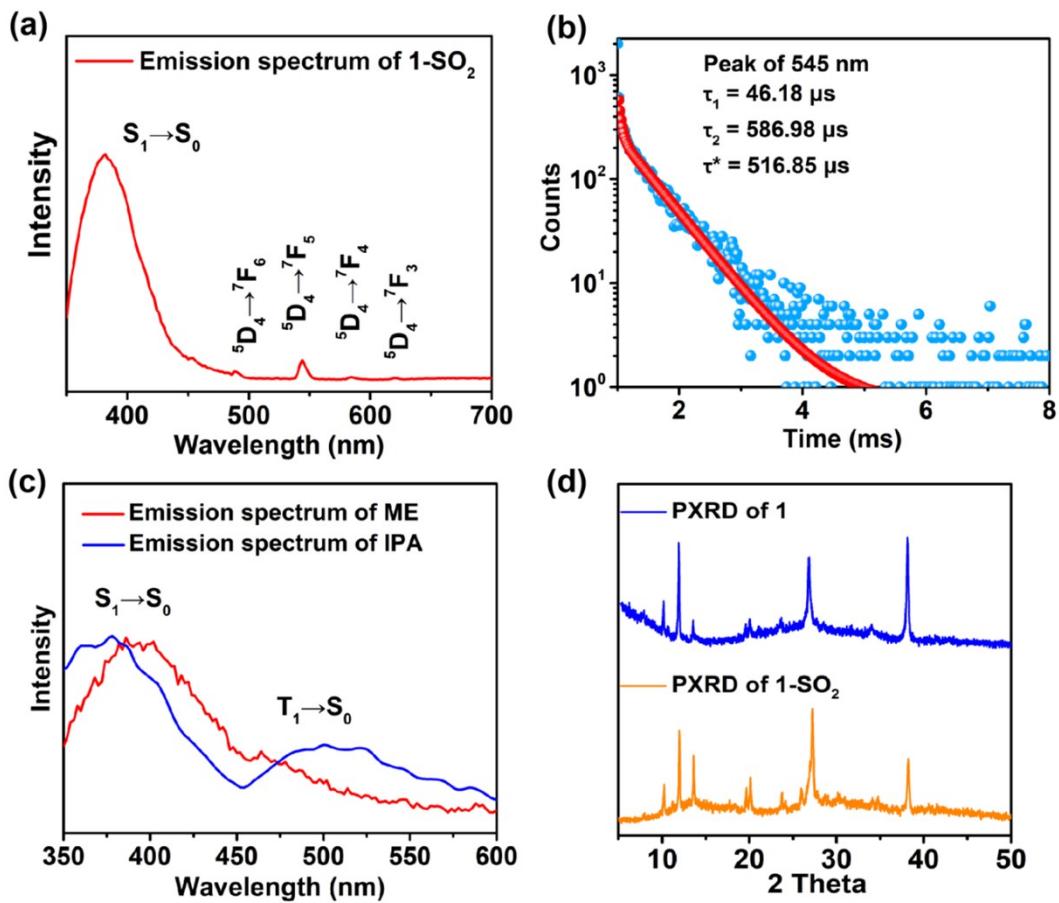


Fig. S11. (a) Emission spectrum of 1-SO_2 ($C_{\text{SO}_2} = 10^{-2} \text{ M}$). (b) Decay lifetime of 545 nm emission peak of **1** ($\lambda_{\text{ex}} = 290 \text{ nm}$). (c) Emission spectra of ME and IPA powders. (d) PXRD patterns of **1** and 1-SO_2 .

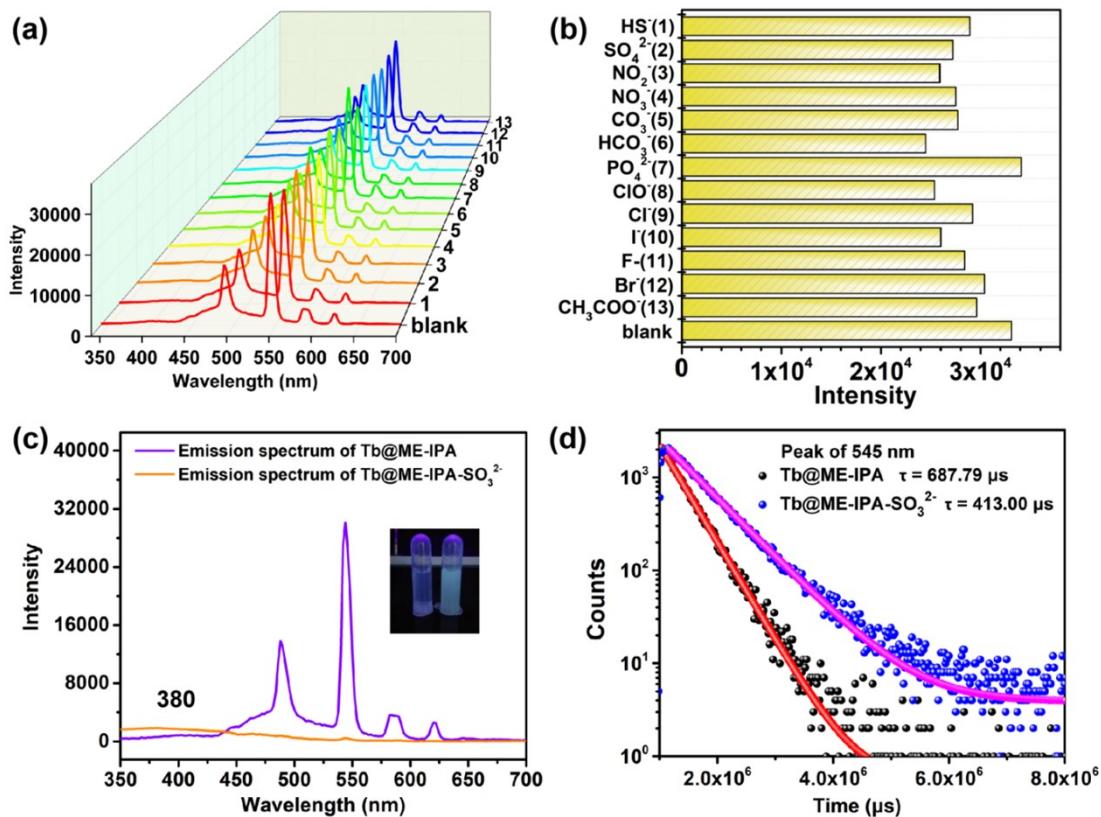


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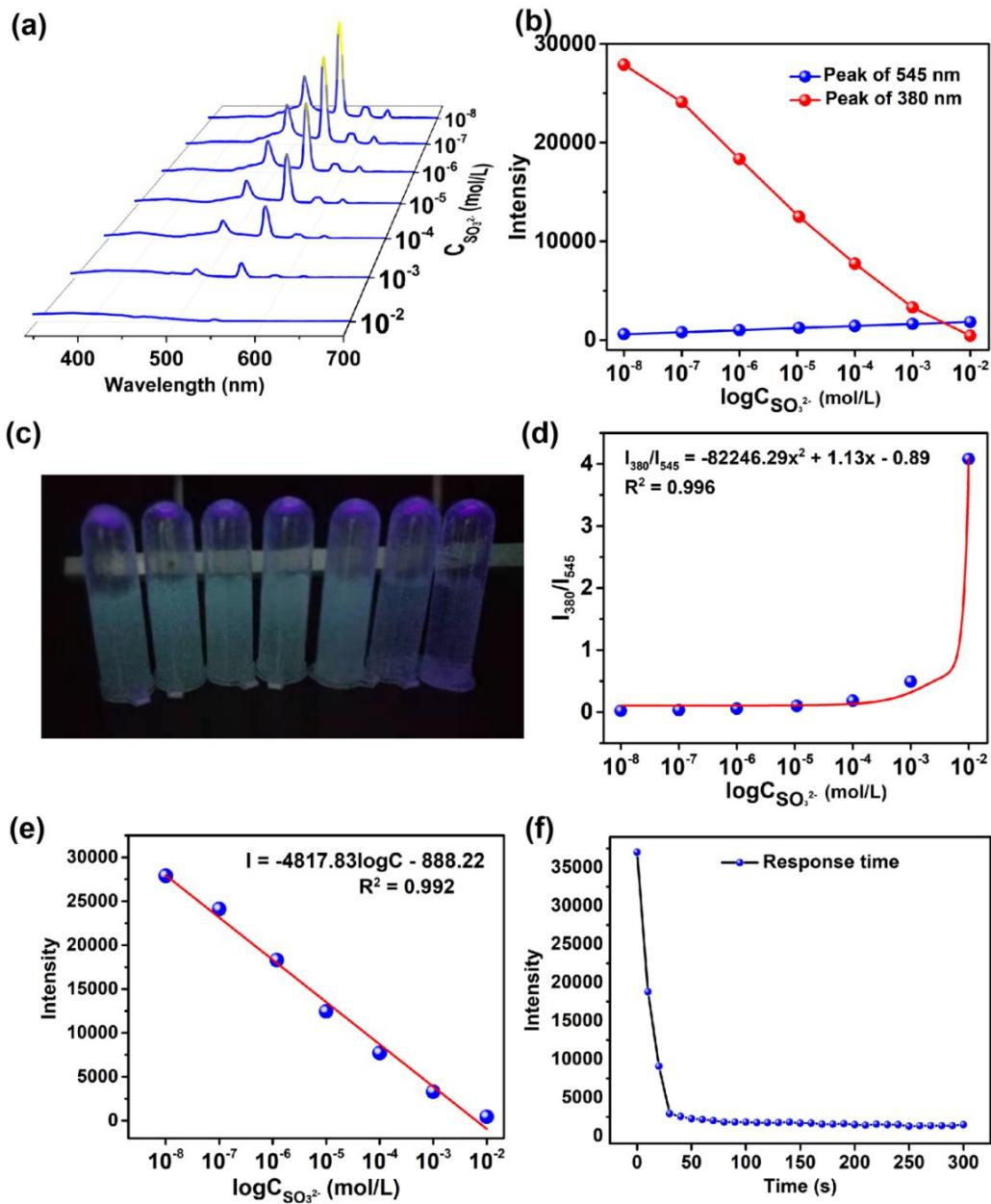


Fig. S13. (a) Emission spectra of Tb@ME-IPA in various SO_3^{2-} solutions with a successive concentration ($C = 10^{-8}\text{-}10^{-2} \text{ M}$) ($\lambda_{\text{ex}} = 290 \text{ nm}$). (b) Dependence of emission intensity of 545 and 380 nm peaks on SO_3^{2-} concentration. (c) Emitting pictures of Tb@ME-IPA in various SO_3^{2-} solutions with a successive concentration ($C = 10^{-8}\text{-}10^{-2} \text{ M}$) ($\lambda_{\text{ex}} = 290 \text{ nm}$). (d) Dependence of emission intensity ratio of 380 and 545 nm peaks on SO_3^{2-} concentration ($C = 10^{-8}\text{-}10^{-2} \text{ M}$) (e) Calibration curves of Tb@ME-IPA toward SO_3^{2-} in the concentration range of $10^{-8}\text{-}10^{-2} \text{ M}$. (f) Response time of Tb@ME-IPA toward SO_3^{2-} .

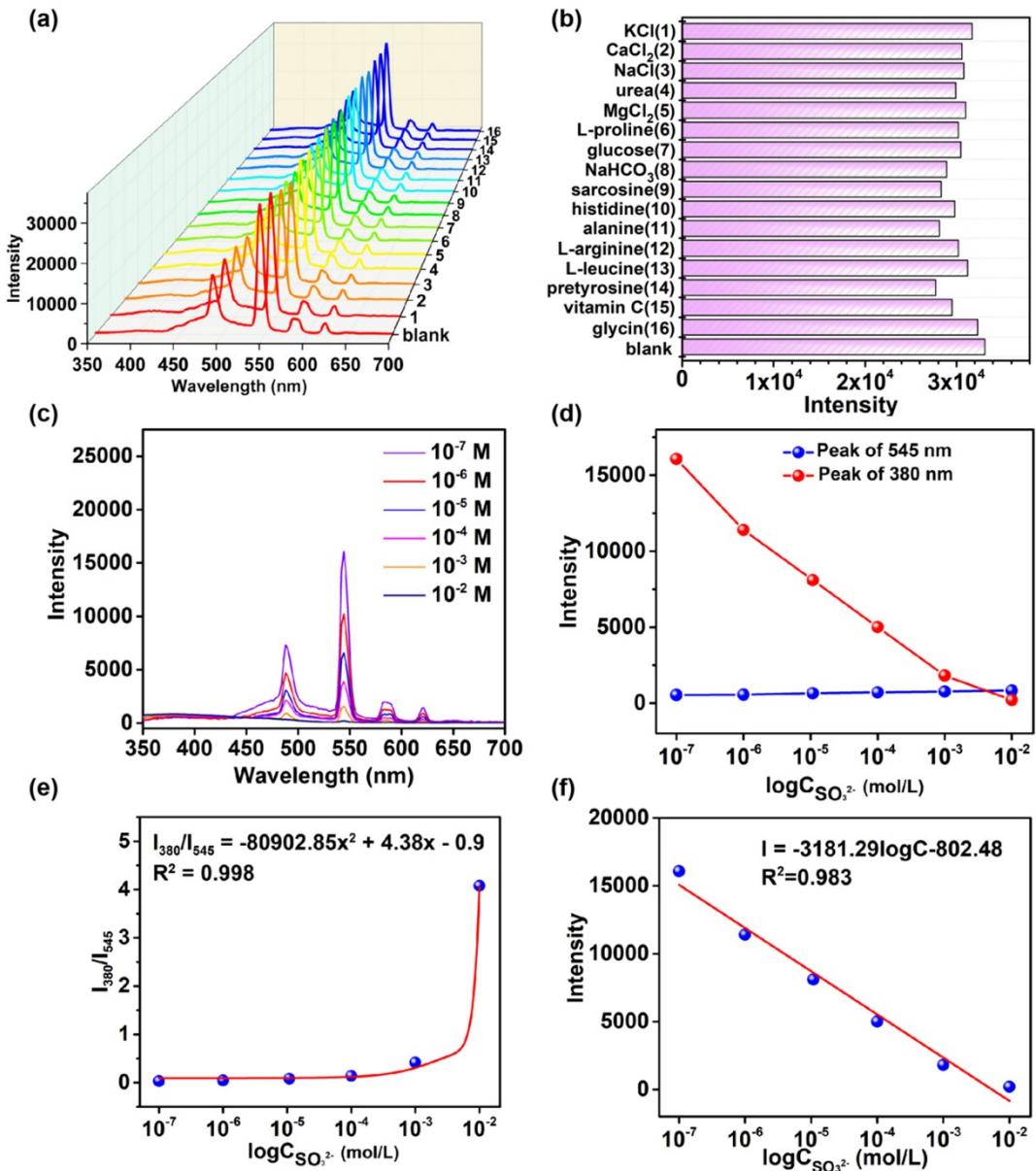


Fig. S14. (a) Emission spectra of Tb@ME-IPA in various serum components ($C = 10^{-2}$ M) ($\lambda_{ex} = 290$ nm). (b) Histogram of 545 nm emission peak of Tb@ME-IPA in various serum components ($C = 10^{-2}$ M). (c) Emission spectra of Tb@ME-IPA in serum system in various SO₃²⁻ solutions with a successive concentration ($C = 10^{-8}$ –10⁻² M) ($\lambda_{ex} = 290$ nm). (d) Dependence of emission intensity of 545 and 380 nm peaks on SO₃²⁻ concentration. (e) Dependence of emission intensity ratio of 380 and 545 nm peaks on SO₃²⁻ concentration (10⁻⁷–10⁻² M). (f) Calibration curves of Tb@ME-IPA toward SO₃²⁻ in the concentration range of 10⁻⁷–10⁻² M.

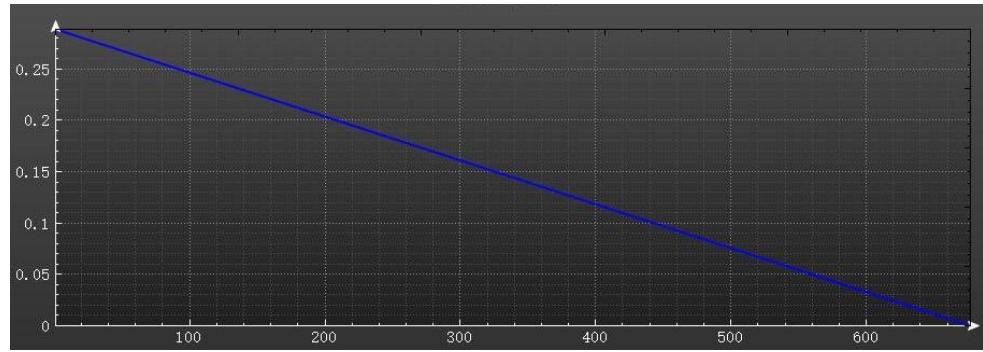


Fig. S15. Network training curve of the BPNN.

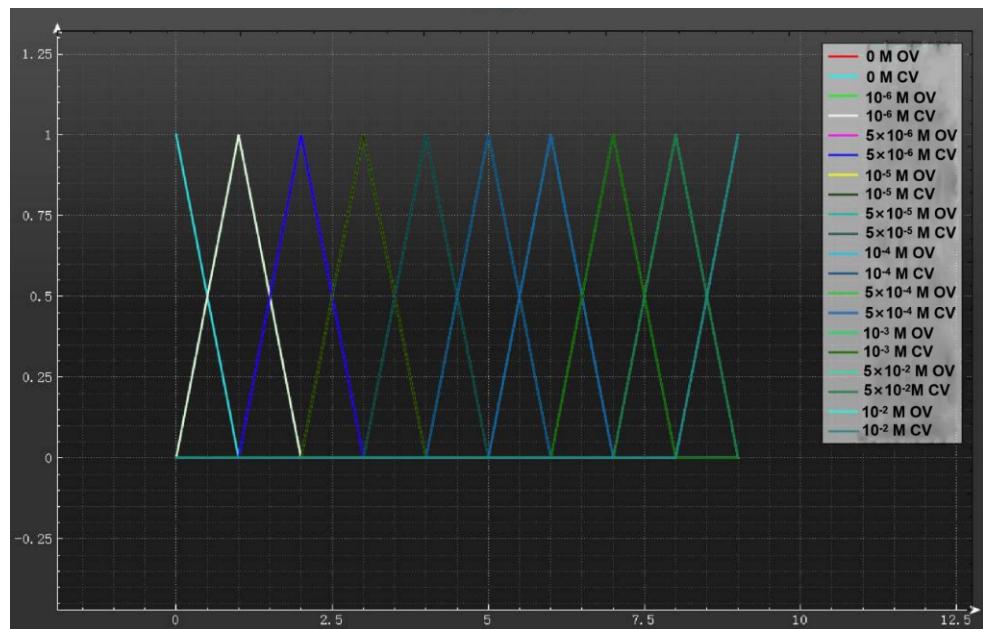


Fig. S16. Deviation curve of the BPNN (OV: original value; CV: calculated value).

In Fig. S16, there are two type of curves respectively representing original value (OV) and calculated value (CV). All curves of OV are overlapped well with the curves of CV, which indicating the low deviation between original and calculated values of output information. Therefore, all curves of OV can not be seen and all curves of CV can only be seen.

Table S1. The reaction equations for preparation of various gases.

NO.	Gas	Reaction equation
1	N ₂	NH ₄ Cl + NaNO ₂ = NaCl + 2H ₂ O + N ₂ ↑
2	O ₂	H ₂ O ₂ = 2 H ₂ O + O ₂ ↑ (MnO ₂ as catalyst)
3	CO ₂	Na ₂ CO ₃ + H ₂ SO ₄ (conc.) = 2Na ₂ SO ₄ + CO ₂ ↑ + H ₂ O
4	SO ₂	Na ₂ SO ₃ + H ₂ SO ₄ (conc.) = Na ₂ SO ₄ + H ₂ O + SO ₂ ↑
5	H ₂ S	Na ₂ S + H ₂ SO ₄ (conc.) = Na ₂ SO ₄ + H ₂ S↑
6	CO	HCOOH = CO↑ + H ₂ O (H ₂ SO ₄ as catalyst)
7	NO	3Na ₂ SO ₃ + 2HNO ₃ (dil.) = 3Na ₂ SO ₄ + 2NO↑ + H ₂ O
8	NO ₂	2KI + 4HNO ₃ (conc.) = I ₂ + 2NO ₂ ↑ + 2KNO ₃ + 2H ₂ O
9	H ₂	Zn + H ₂ SO ₄ = ZnSO ₄ + H ₂ ↑
10	CH ₄	CH ₃ COONa + NaOH =△= Na ₂ CO ₃ + CH ₄ ↑ (CaO as catalyst)
11	NH ₃	volatilization of ammonia
12	C ₇ H ₈	volatilization of toluene
13	CH ₃ OH	volatilization of methanol
14	C ₂ H ₅ OH	volatilization of ethanol
15	CH ₃ COCH ₃	volatilization of acetone

Table S2. Element contents of C, N, O, Tb in EDX energy spectrum **1** and C, N, O, S, Tb in EDX energy spectrum 1-SO₂.

1		1-SO ₂	
Elements	W _t %	Elements	W _t %
C	53.52	C	45.71
N	36.52	N	33.97
O	8.39	O	16.36
Tb	1.57	S	2.64
		Tb	1.32

Table S3. Summary of decay lifetime of **1**, 1-SO₂, Tb@ME-IPA, and Tb@ME-IPA-SO₃²⁻.

Sample	λ_{ex} (nm)	λ_{em} (nm)	τ_1 (μs)	A_1	Percentag		Percentag		τ^*	χ^2
					e (%)	τ_2 (μs)	A_2	e (%)		
1	290	545	597.43	1510.98	61.42	1076.77	526.56	38.58	790.24	1.457
1-SO ₂	290	545	46.18	496.88	12.97	586.98	262.36	87.03	516.85	1.070
Tb@ME-IPA	290	545	687.79	2019.57	100.00	-	-	-	-	1.390
Tb@ME-IPA-SO ₃ ²⁻	290	545	413.00	2181.39	100.00	-	-	-	-	1.181

Table S4. Summary of emission transitions and experimental energy gaps of ME-IPA and Tb³⁺ ions.

	Transitions	Wavelength (nm)	Energy gap (eV)
ME-IPA	S ₁ →S ₀	359	3.45
	T ₁ →S ₀	486	2.55
	⁵ D ₄ → ⁷ F _K	488	2.54
Tb ³⁺	⁵ D ₄ → ⁷ F _K	545	2.28
	⁵ D ₄ → ⁷ F _K	583	2.13
	⁵ D ₄ → ⁷ F _K	621	2.00

Table S5. Summary of R.G.B. of emitting color of **1** exposed in various SO₂ concentration (10⁻⁶-10⁻² M).

Concentration n	10 ⁻⁶	10 ⁻⁵	10 ⁻⁴	10 ⁻³	10 ⁻²
Color	PaleGreen1	DarkSeaGreen3	lavender	SlateBlue3	SlateBlue4
Picture					
R.G.B	154 255 154	155 205 155	230 230 250	105 89 205	71 60 139

Concentration n	5×10 ⁻⁶	5×10 ⁻⁵	5×10 ⁻⁴	5×10 ⁻³	0
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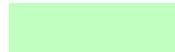
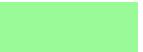
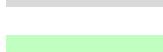
Color	SeaGreen1	DarkSeaGreen 1	MediumPurple 1	Blue4	PaleGreen
Picture					
R.G.B	84 255 159	193 255 193	171 130 255	0 0 139	152 251 152

Table S6. Summary of input and output information during the training of BPNN for SO₂ detection.

Picture	Input (R.G.B value)			Output [Concentration of SO ₂ (M)]									
	R	G	B	0	10 ⁻⁶	5×10 ⁻⁶	10 ⁻⁵	5×10 ⁻⁶	10 ⁻⁴	5×10 ⁻⁶	10 ⁻³	5×10 ⁻⁶	10 ⁻²
	152	251	152	1	0	0	0	0	0	0	0	0	0
	154	255	154	0	1	0	0	0	0	0	0	0	0
	84	255	159	0	0	1	0	0	0	0	0	0	0
	155	205	155	0	0	0	1	0	0	0	0	0	0
	193	255	193	0	0	0	0	1	0	0	0	0	0
	230	230	250	0	0	0	0	0	1	0	0	0	0
	171	130	255	0	0	0	0	0	0	1	0	0	0
	105	89	205	0	0	0	0	0	0	0	1	0	0
	0	0	139	0	0	0	0	0	0	0	0	1	0
	71	60	139	0	0	0	0	0	0	0	0	0	1

In Table S6, all data is used to training the BPNN. The R.G.B values of every color as input information are inputted in the input column of the BPNN. Various “0” and “1” inputted into the output column of the BPNN, in which “0” represents the false SO₂ concentration, and “1” represents the correct SO₂ concentration. All data is used to train the BPNN.

Table S7. Network structure information.

Network structure information				
Input layer	3 neurons	1	Paranoid	
Hidden layer 1	5 neurons	1	Paranoid	
Output layer	10neurons			
Network type	FANN_NETTYPE_LAYER			
Training function	FANN_TRAIN_RPROP			
Error function	FANN_ERRORFUNC_LINEAR			
Termination function	FANN_STOPFUNC_MSE			
Hidden layer excitation function	FANN_SIGMOID_SYMMETRIC			
Output layer excitation function	FANN_SIGMOID_SYMMETRIC			
Network weight value				
Arrangement	Wire number	Output point (n)	Input point (m)	Weight value (W)
1	0	0	4	-2.17058
	1	1	4	2.57524
	2	2	4	0.698852
	3	3	4	-1.39816
	4	0	5	-43.6209
	5	1	5	-450.595
	6	2	5	0.0045888
	7	3	5	-1448
	8	0	6	-0.119756
	9	1	6	0.562446
	10	2	6	2.00202
	11	3	6	-2.59579
	12	0	7	6.57045
	13	1	7	-1.05856
	14	2	7	5.28074
2	15	3	7	2.98667
	16	0	8	-2.73271
	17	1	8	0.0701685
	18	2	8	2.79813
	19	3	8	2.20223
	20	4	10	31.5016
	21	5	10	10.9008
	22	6	10	2.08634
	23	7	10	-140.654
	24	8	10	-231.037
	25	9	10	-20.8311
	26	4	11	372.743

27	5	11	1.01869
28	6	11	-0.166004
29	7	11	106.199
30	8	11	-170.102
31	9	11	-6.412
32	4	12	1500
33	5	12	1500
34	6	12	1500
35	7	12	189.882
36	8	12	1500
37	9	12	1500
38	4	13	-155.524
39	5	13	4.05623
40	6	13	0.180367
41	7	13	40.7606
42	8	13	-155.069
43	9	13	-81.8848
44	4	14	278.475
45	5	14	25.7603
46	6	14	5.32007
47	7	14	144.396
48	8	14	-18.4874
49	9	14	-12.1015
50	4	15	1500
51	5	15	1500
52	6	15	1500
53	7	15	1204.98
54	8	15	940.559
55	9	15	1203.07
56	4	16	-160.791
57	5	16	39.0143
58	6	16	105.367
59	7	16	1.56348
60	8	16	15.5595
61	9	16	-24.122
62	4	17	-6.50918
63	5	17	9.84273
64	6	17	-72.4171
65	7	17	17.6102
66	8	17	29.5826
67	9	17	-87.4224
68	4	18	-26.4926
69	5	18	136.401
70	6	18	0.223098

71	7	18	-44.1377
72	8	18	158.281
73	9	18	-23.7568
74	4	19	-44.9046
75	5	19	25.2329
76	6	19	0.697594
77	7	19	-64.528
78	8	19	-95.4034
79	9	19	-18.2412

Input / output column coefficients for manual calculation

Listing	Minimum	Maximum
R	0	242.105
G	0	268.421
B	132.05	268.421
0 M	0	1
0.000001 M	0	1
0.000005 M	0	1
0.00001 M	0	1
0.00005 M	0	1
0.0001 M	0	1
0.0005 M	0	1
0.001 M	0	1
0.005 M	0	1
0.01 M	0	1

Deviation statistics: mean variance

Listing	All rows	Calculation line	Test line
0 M	6.6085e-10	6.6085e-10	0
0.000001 M	2.8365e-10	2.8365e-10	0
0.000005 M	2.5e-14	2.5e-14	0
0.00001 M	0	0	0
0.00005 M	0	0	0
0.0001 M	0	0	0
0.0005 M	0	0	0
0.001 M	6.825e-12	6.825e-12	0
0.005 M	0	0	0
0.01 M	0	0	0

Table S8. The summary of mean square error (MSE), original value (OV), calculated value (CV), variance (Var.)

1	Input item			0 M (MSE = 6.6085e-10)			0.000001 M (MSE = 2.8365e-10)			0.000005 M (MSE = 2.5e-14)			0.00001 M (MSE = 0)		
	R	G	B	OV			OV			OV			OV		
				CV.	Var.	.	CV.	Var.	.	CV.	Var.	.	CV.	Var.	.
3	152	251	152	1	0.999934	4.356e-09	0	3.25e-05	1.05625e-09	0	0	0	0	0	0
4	154	255	154	0	4.65e-05	2.16225e-09	1	0.999958	1.764e-09	0	0	0	0	0	0
5	84	255	159	0	0	0	0	2e-06	4e-12	1	1	0	0	0	0
6	155	205	155	0	0	0	0	0	0	0	0	0	1	1	0
7	193	255	193	0	0	0	0	3.5e-06	1.225e-11	0	0	0	0	0	0
8	230	230	250	0	0	0	0	0	0	0	5e-07	2.5e-13	0	0	0
9	171	130	255	0	0	0	0	0	0	0	0	0	0	0	0
10	105	89	205	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	139	0	0	0	0	0	0	0	0	0	0	0	0
12	71	60	139	0	9.5e-06	9.025e-11	0	0	0	0	0	0	0	0	0

1	0.00005 M(MSE = 0)			0.0001 M(MSE = 0)			0.0005 M(MSE = 0)			0.001 M(MSE = 6.825e-12)			0.005 M(MSE = 0)			0.01 M(MSE = 0)		
	OV.	CV.	Var.	OV.	CV.	Var.	OV.	CV.	Var.	OV.	CV.	Var.	OV.	CV.	Var.			
													.	.	.			
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0			
7	1	1	0	0	0	0	0	0	0	1.5e-06	2.25e-12	0	0	0	0			
8	0	0	0	1	1	0	0	0	0	0	0	0	0	0	0			
9	0	0	0	0	0	1	1	0	0	4e-06	1.6e-11	0	0	0	0			
10	0	0	0	0	0	0	0	0	1	0.999993	4.9e-11	0	0	0	0			
11	0	0	0	0	0	0	0	0	0	1e-06	1e-12	1	1	0	0			
12	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0			

In Table S8, all data is utilized to test the BPNN. The R.G.B values of every color as input information are inputted in the input column of the BPNN. Through the BPNN calculation, various values (0-1) can be outputted, in which the values close to “0” represents the false SO₂ concentration, the values close to “1” represents the correct SO₂ concentration. By comparing the OV with CV, the variance can be obtained, which suggests that the BPNN has a good accuracy for detecting SO₂ concentration.

Table S9. The summary of input and output information in real batch calculation during the test of BPNN.

Input data			Output data									
R	G	B	0 M	0.00001 M	0.00005 M	0.0001 M	0.0005 M	0.001 M	0.005 M	0.05 M	0.1 M	
152	251	152	0.999934	3.25864e-05	0	0	0	0	1.44329e-15	0	1.50328e-09	
154	255	154	4.66943e-05	0.999958	0	0	0	0	1.16573e-14	0	3.747e-14	
84	255	159	5.66547e-13	1.76799e-06	1	0	0	0	1.53211e-14	5.55112e-17	0	
155	205	155	0	0	0	1	0	0	2.66377e-11	0	1.87311e-12	
193	255	193	0	3.37203e-06	0	5.55112e-17	1	0	0	1.71061e-06	0	0
230	230	250	0	0	5.81046e-07	0	5.55112e-17	1	2.20176e-08	3.34388e-12	0	0
171	130	255	0	0	0	0	0	4.35348e-10	1	3.93021e-06	5.55112e-17	0
105	89	205	0	0	0	0	0	0	4.24601e-09	0.999993	0	0
0	0	139	0	0	0	0	0	0	9.54616e-10	1.14786e-06	1	8.37655e-10
71	60	139	9.49636e-06	0	0	0	0	0	1.89536e-11	2.9306e-12	1.11022e-16	1

In Table S9, all data is utilized to test the BPNN. The R.G.B values of every color as input information are inputted in the input column of the BPNN. Through the BPNN calculation, various values (0-1) can be acquired, in which the values close to "0" represents the false SO₂ concentration, and the values close to 1 represents the correct SO₂ concentration.

Table S10. The matlab code of this BPNN.

Matlab code
<pre> function [f00,f01,f02,f03,f04,f05,f06,f07,f08,f09] = MPredict(f10,f11,f12) f10 = (f10 - (0 + 242.1052631578947398) / 2.0) /(242.1052631578947398 - (0 + 242.1052631578947398) / 2.0); f11 = (f11 - (0 + 268.4210526315789593) / 2.0) /(268.4210526315789593 - (0 + 268.4210526315789593) / 2.0); f12 = (f12 - (132.0499999999999829 + 268.4210526315789593) / 2.0) /(268.4210526315789593 - (132.0499999999999829 + 268.4210526315789593) / 2.0); fWei0 = -2.17058; fWei1 = 2.57524; fWei2 = 0.698852; fWei3 = -1.39816; fWei4 = -43.6209; fWei5 = -450.595; fWei6 = 0.0045888; fWei7 = -1448; fWei8 = -0.119756; fWei9 = 0.562446; fWei10 = 2.00202; fWei11 = -2.59579; fWei12 = 6.57045; fWei13 = -1.05856; fWei14 = 5.28074; fWei15 = 2.98667; fWei16 = -2.73271; </pre>

```
fWei17 = 0.0701685;
fWei18 = 2.79813;
fWei19 = 2.20223;
fWei20 = 31.5016;
fWei21 = 10.9008;
fWei22 = 2.08634;
fWei23 = -140.654;
fWei24 = -231.037;
fWei25 = -20.8311;
fWei26 = 372.743;
fWei27 = 1.01869;
fWei28 = -0.166004;
fWei29 = 106.199;
fWei30 = -170.102;
fWei31 = -6.412;
fWei32 = 1500;
fWei33 = 1500;
fWei34 = 1500;
fWei35 = 189.882;
fWei36 = 1500;
fWei37 = 1500;
fWei38 = -155.524;
fWei39 = 4.05623;
fWei40 = 0.180367;
fWei41 = 40.7606;
fWei42 = -155.069;
fWei43 = -81.8848;
fWei44 = 278.475;
fWei45 = 25.7603;
fWei46 = 5.32007;
fWei47 = 144.396;
fWei48 = -18.4874;
fWei49 = -12.1015;
fWei50 = 1500;
fWei51 = 1500;
fWei52 = 1500;
fWei53 = 1204.98;
fWei54 = 940.559;
fWei55 = 1203.07;
fWei56 = -160.791;
fWei57 = 39.0143;
fWei58 = 105.367;
fWei59 = 1.56348;
fWei60 = 15.5595;
fWei61 = -24.122;
fWei62 = -6.50918;
fWei63 = 9.84273;
fWei64 = -72.4171;
fWei65 = 17.6102;
fWei66 = 29.5826;
fWei67 = -87.4224;
fWei68 = -26.4926;
fWei69 = 136.401;
fWei70 = 0.223098;
fWei71 = -44.1377;
fWei72 = 158.281;
fWei73 = -23.7568;
```

```
fWei74 = -44.9046;
fWei75 = 25.2329;
fWei76 = 0.697594;
fWei77 = -64.528;
fWei78 = -95.4034;
fWei79 = -18.2412;
f0 = f10;
f1 = f11;
f2 = f12;
f3 = 1.0;
f4 = 0.0;
f5 = 0.0;
f6 = 0.0;
f7 = 0.0;
f8 = 0.0;
f4 = f4 + f0 * fWei0;
f4 = f4 + f1 * fWei1;
f4 = f4 + f2 * fWei2;
f4 = f4 + f3 * fWei3;
f4 = f4 * 0.5;
f4 = (2.0 / (1.0 + exp(-2.0 * f4))- 1.0);
f5 = f5 + f0 * fWei4;
f5 = f5 + f1 * fWei5;
f5 = f5 + f2 * fWei6;
f5 = f5 + f3 * fWei7;
f5 = f5 * 0.5;
f5 = (2.0 / (1.0 + exp(-2.0 * f5))- 1.0);
f6 = f6 + f0 * fWei8;
f6 = f6 + f1 * fWei9;
f6 = f6 + f2 * fWei10;
f6 = f6 + f3 * fWei11;
f6 = f6 * 0.5;
f6 = (2.0 / (1.0 + exp(-2.0 * f6))- 1.0);
f7 = f7 + f0 * fWei12;
f7 = f7 + f1 * fWei13;
f7 = f7 + f2 * fWei14;
f7 = f7 + f3 * fWei15;
f7 = f7 * 0.5;
f7 = (2.0 / (1.0 + exp(-2.0 * f7))- 1.0);
f8 = f8 + f0 * fWei16;
f8 = f8 + f1 * fWei17;
f8 = f8 + f2 * fWei18;
f8 = f8 + f3 * fWei19;
f8 = f8 * 0.5;
f8 = (2.0 / (1.0 + exp(-2.0 * f8))- 1.0);
f9 = 1.0;
f10 = 0.0;
f11 = 0.0;
f12 = 0.0;
f13 = 0.0;
f14 = 0.0;
f15 = 0.0;
f16 = 0.0;
f17 = 0.0;
f18 = 0.0;
f19 = 0.0;
f10 = f10 + f4 * fWei20;
```

```
f10 = f10 + f5 * fWei21;
f10 = f10 + f6 * fWei22;
f10 = f10 + f7 * fWei23;
f10 = f10 + f8 * fWei24;
f10 = f10 + f9 * fWei25;
f10 = f10 * 0.5;
f10 = (2.0 / (1.0 + exp(-2.0 * f10))- 1.0);
f11 = f11 + f4 * fWei26;
f11 = f11 + f5 * fWei27;
f11 = f11 + f6 * fWei28;
f11 = f11 + f7 * fWei29;
f11 = f11 + f8 * fWei30;
f11 = f11 + f9 * fWei31;
f11 = f11 * 0.5;
f11 = (2.0 / (1.0 + exp(-2.0 * f11))- 1.0);
f12 = f12 + f4 * fWei32;
f12 = f12 + f5 * fWei33;
f12 = f12 + f6 * fWei34;
f12 = f12 + f7 * fWei35;
f12 = f12 + f8 * fWei36;
f12 = f12 + f9 * fWei37;
f12 = f12 * 0.5;
f12 = (2.0 / (1.0 + exp(-2.0 * f12))- 1.0);
f13 = f13 + f4 * fWei38;
f13 = f13 + f5 * fWei39;
f13 = f13 + f6 * fWei40;
f13 = f13 + f7 * fWei41;
f13 = f13 + f8 * fWei42;
f13 = f13 + f9 * fWei43;
f13 = f13 * 0.5;
f13 = (2.0 / (1.0 + exp(-2.0 * f13))- 1.0);
f14 = f14 + f4 * fWei44;
f14 = f14 + f5 * fWei45;
f14 = f14 + f6 * fWei46;
f14 = f14 + f7 * fWei47;
f14 = f14 + f8 * fWei48;
f14 = f14 + f9 * fWei49;
f14 = f14 * 0.5;
f14 = (2.0 / (1.0 + exp(-2.0 * f14))- 1.0);
f15 = f15 + f4 * fWei50;
f15 = f15 + f5 * fWei51;
f15 = f15 + f6 * fWei52;
f15 = f15 + f7 * fWei53;
f15 = f15 + f8 * fWei54;
f15 = f15 + f9 * fWei55;
f15 = f15 * 0.5;
f15 = (2.0 / (1.0 + exp(-2.0 * f15))- 1.0);
f16 = f16 + f4 * fWei56;
f16 = f16 + f5 * fWei57;
f16 = f16 + f6 * fWei58;
f16 = f16 + f7 * fWei59;
f16 = f16 + f8 * fWei60;
f16 = f16 + f9 * fWei61;
f16 = f16 * 0.5;
f16 = (2.0 / (1.0 + exp(-2.0 * f16))- 1.0);
f17 = f17 + f4 * fWei62;
f17 = f17 + f5 * fWei63;
```

```
f17 = f17 + f6 * fWei64;
f17 = f17 + f7 * fWei65;
f17 = f17 + f8 * fWei66;
f17 = f17 + f9 * fWei67;
f17 = f17 * 0.5;
f17 = (2.0 / (1.0 + exp(-2.0 * f17))- 1.0);
f18 = f18 + f4 * fWei68;
f18 = f18 + f5 * fWei69;
f18 = f18 + f6 * fWei70;
f18 = f18 + f7 * fWei71;
f18 = f18 + f8 * fWei72;
f18 = f18 + f9 * fWei73;
f18 = f18 * 0.5;
f18 = (2.0 / (1.0 + exp(-2.0 * f18))- 1.0);
f19 = f19 + f4 * fWei74;
f19 = f19 + f5 * fWei75;
f19 = f19 + f6 * fWei76;
f19 = f19 + f7 * fWei77;
f19 = f19 + f8 * fWei78;
f19 = f19 + f9 * fWei79;
f19 = f19 * 0.5;
f19 = (2.0 / (1.0 + exp(-2.0 * f19))- 1.0);
f00 = f10;
f01 = f11;
f02 = f12;
f03 = f13;
f04 = f14;
f05 = f15;
f06 = f16;
f07 = f17;
f08 = f18;
f09 = f19;
f00 = f00 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f01 = f01 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f02 = f02 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f03 = f03 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f04 = f04 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f05 = f05 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f06 = f06 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f07 = f07 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f08 = f08 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
f09 = f09 * (1 - (0 + 1) / 2.0) + (0 + 1) / 2.0;
```
