Electronic Supplementary Material (ESI) for Soft Matter.

Electronic Supplementary Information

Novel multi-analytes responsive ionic supramolecular gels based on pyridinium functionalized-naphthalimide

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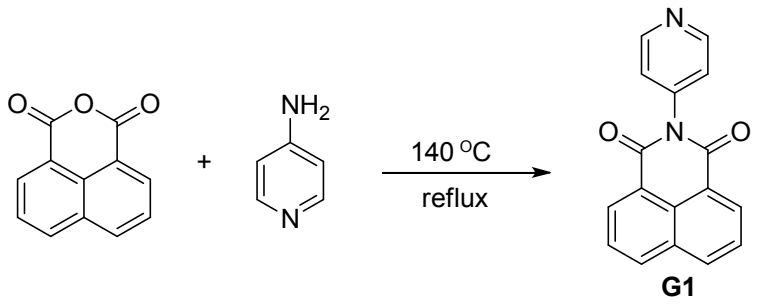
Materials and physical methods

All anions were used as tetrabutylammonium salts, which were purchased from Alfa Aesar and used as received. All metal ions were prepared from the perchlorate salts. Other reagents used in the study were of analytical grade. Fresh double distilled water was used throughout the experiment. All other reagents and solvents were commercially available at analytical grade and were used without further purification. ^{1}H NMR spectra were recorded on Mercury-400BB spectrometer (400MHz) and Bruker Digital RF spectrometer (300MHz). ^{1}H chemical shifts are reported in ppm downfield from tetramethylsilane (TMS, ™ scale with the solvent resonances as internal standards). Mass spectra were performed on a Bruker Esquire 3000 plus mass spectrometer (Bruker-FranzenAnalytik GmbH Bremen, Germany) equipped with ESI interface and ion trap analyzer. The X-ray diffraction analysis (XRD) was performed on a Rigaku D/Max-2400 X-Ray Diffractometer. The morphologies and sizes of the xerogels were characterized using field emission scanning electron microscopy (FE-SEM, JSM-6701F) at an accelerating voltage of 8 kV. The infrared spectra were performed on a Digilab FTS-3000 Fourier transform-infrared spectrophotometer. Melting points were measured on an X-4 digital melting-point apparatus (uncorrected). Ultraviolet-visible (UV-vis) spectra were recorded on a Shimadzu UV-2550 spectrometer. Fluorescence spectra were recorded on a Shimadzu RF-5301PC spectrofluorophotometer.

2. Synthesis and characterizations of compound G1.



Scheme S1 The synthesis of compound **G1**.

Synthesis of compound G1

1,8-Naphthalimide (1.98 g, 10 mmol) and 4-aminopyridine (0.95 g, 10 mmol) was suspended in anhydrous DMF (75 mL) and heated to 140 °C under a N_2 atmosphere in a 100 mL reaction flask equipped with a stir bar. The reaction mixture was then heated under reflux in an N_2 atmosphere overnight. Afterwards, the solution was cooled to room temperature, the mixture was poured into H_2O (15 mL). The precipitate was collected by filtration, washed with ethanol (20 mL × 3) and then dried in vacuum; give a beige powder compound **G1**. Yield: 1.87g (68.2%). m.p.>300 °C. ^{1}H NMR (400 MHz, DMSO-d_6, Fig. S1): δ 8.73 (d, J = 4.8 Hz, 2H), 8.53 (t, J = 6.8 HZ, 4H), 7.93 (t, J = 8.0 Hz, 2H, ArH), 7.53 (m, 2H, ArH). ESI-MS calcd for $[C_{17}H_{10}O_2N_2 + H]^+$ = 275.08; found: 275.00.

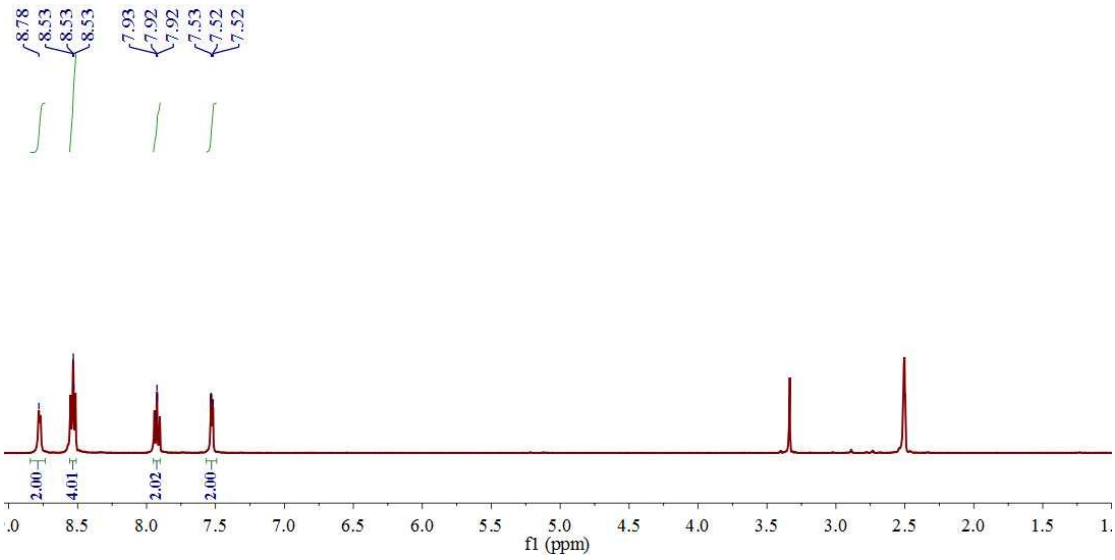


Fig. S1 ^{1}H NMR spectrum of **G1** in DMSO-d_6.

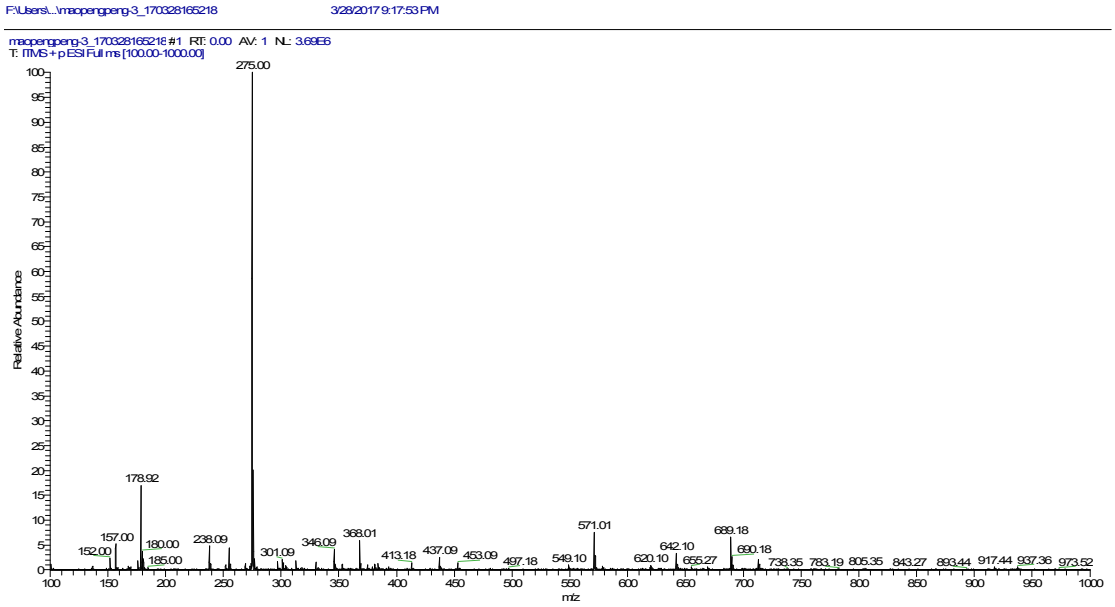


Fig. S2 ESI-MS spectrum of **G1**.

Table S1. Gelation Property of **G1**.

Entry	Solvent	State[a]	CGC[b] (%)	Tgel[c] (^{o}C, wt %)
1	water	P	\	\
2	petroleum ether	P	\	\
3	dichloromethane	P	\	\
4	chloroform	P	\	\
5	ethyl acetate	P	\	\
6	acetone	P	\	\
7	methanol	P	\	\
8	ethanol	P	\	\
9	n-propanol	P	\	\
10	n-butyl alcohol	P	\	\
11	n-Hexanol	P	\	\
12	Acetonitrile	P	\	\
13	DMF	S	\	\
14	DMSO	S	\	\
15	Formic acid	S	\	\
16	acetic acid	P	\	\
17	Propanoic acid	G	4	78
18	n-Butyric acid	G	5	80
19	n-pentanoic acid	G	3	85
20	Caproic acid	G	5	70
21	Heptanoic acid	G	5	63

[a]G, P and S denote gelation, precipitation and solution, respectively. (5%, wt%, 10 mg mL^{-1} = 1.0%)

[b]The critical gelation concentration (5%, wt%, 10 mg mL^{-1} = 1.0%).

[c]The gelation temperature (^{o}C).

Table S2. Gelation Property of **G1** and n-pentanoic acid complex.

Entry	Solvent	State[a]	CGC[b] (%)	Tgel[c] (^{o}C, wt %)
1	water	P	\	\
2	petroleum ether	P	\	\
3	dichloromethane	P	\	\
4	chloroform	P	\	\
5	ethyl acetate	P	\	\
6	acetone	P	\	\
7	methanol	P	\	\
8	ethanol	P	\	\
9	n-propanol	P	\	\
10	n-butyl alcohol	P	\	\
11	n-Hexanol	P	\	\
12	Acetonitrile	P	\	\
13	DMF	P	\	\
14	DMSO	P	\	\

[a]G, P and S denote gelation, precipitation and solution, respectively. (5%, wt%, 10 mg mL^{-1} = 1.0%)

[b]The critical gelation concentration.

[c]The gelation temperature (^{o}C).

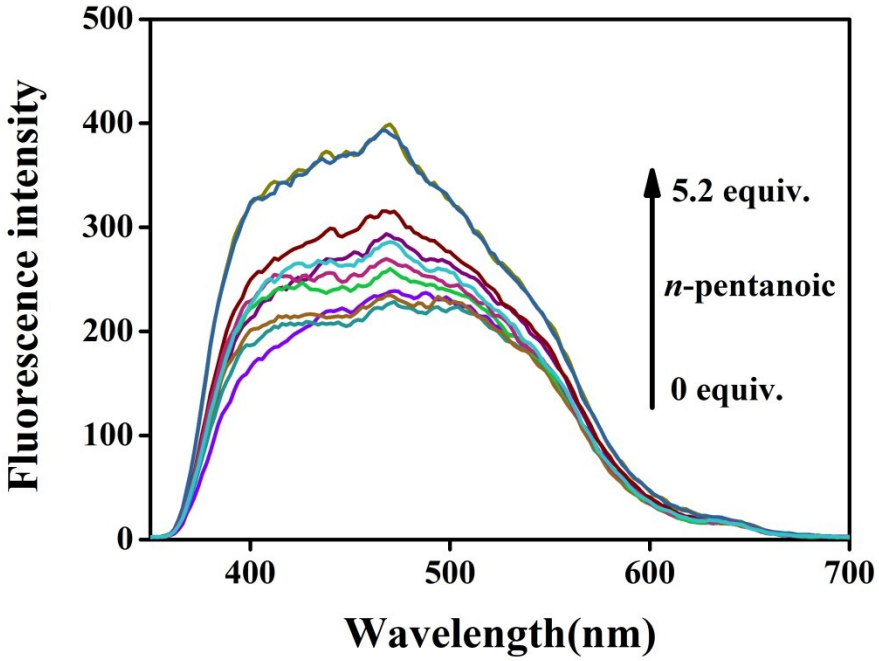


Fig. S3 Fluorescence intensity changes of **G1** DMSO solution (2.0×10^{-4} mol L^{-1}) upon addition of different amounts of *n*-pentanoic (λ_{ex} = 320 nm).

The association constants (Ka) were calculated based on the fluorescent titration curve. Association constants were determined by a nonlinear least squares fit of the data with the following equation as referenced elsewhere. I is the observed the fluorescence intensity of **G1** at the fixed concentrations of *n*-pentanoic. I_{max} and I_{min} are the corresponding maximum and minimum, respectively.

$$\log\frac{I - Imin}{Imax - I} = \log Ka + \log[n - pentanoic]$$

K = 7.89×10^{6} M^{-2}.

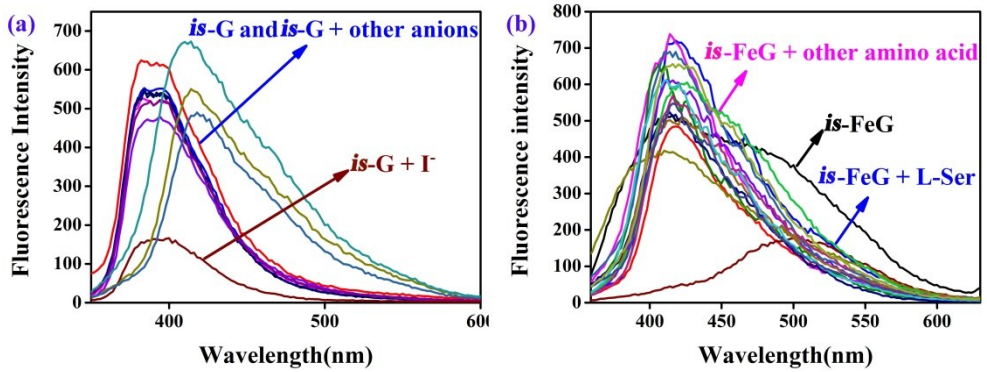


Fig. S4 Fluorescence spectra of (a) ***is*-G** in the presence of various anions; (b) ***is*-FeG** in the presence of various amino acids (λex = 320 nm).

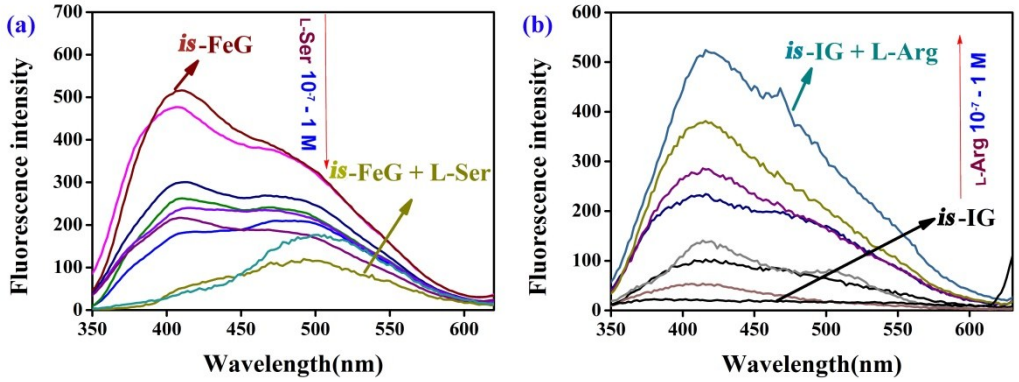


Fig. S5 Fluorescence spectra of (a) ***is*-FeG** with increasing concentration of L-Ser; (b) ***is*-IG** with increasing concentration of L-Arg.

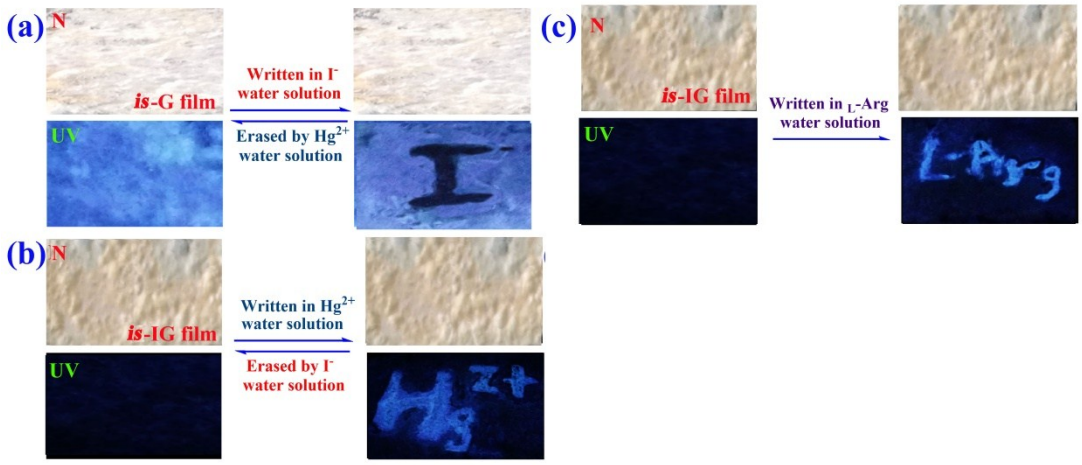


Fig. S6 (a) Photograph of ***is*-G**-based film (obtained from 3% in *n*-pentanoic acid) fluorescently detects I^- in water solution; (b) photograph of ***is*-IG**-based film (obtained from 3% in *n*-pentanoic acid) fluorescently detects Hg^{2+} in water solution, (c) photograph of ***is*-IG**-based film (obtained from 3% in *n*-pentanoic acid) fluorescently detects L-Arg in water solution.

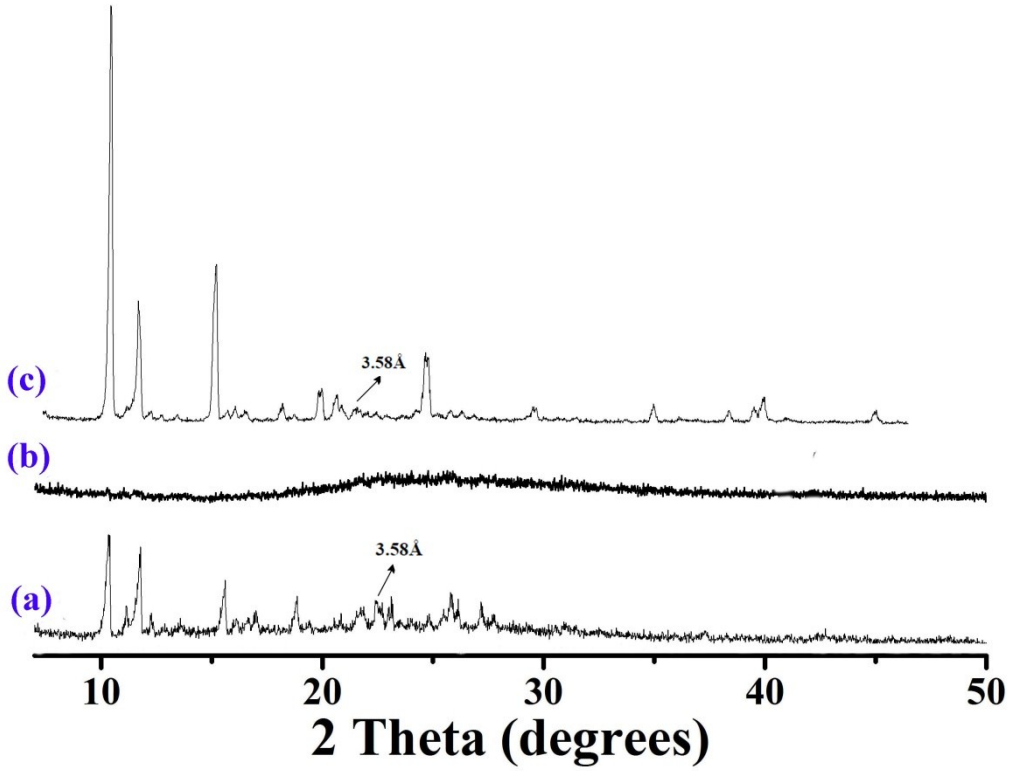


Fig. S7 Powder XRD patterns of (a) ***is*-G**; (b) ***is*-IG;** (c) ***is*-IG** + Hg^{2+}.

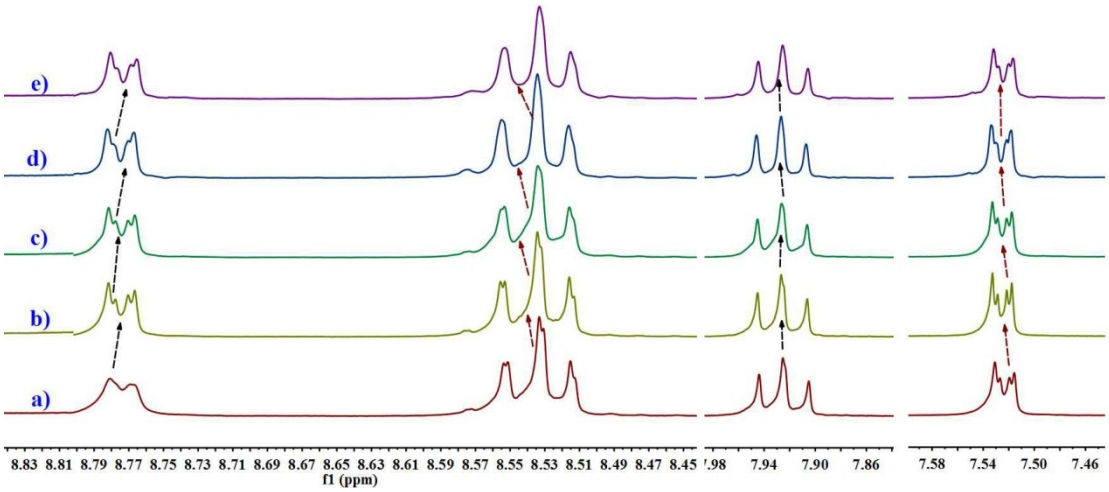


Fig. S8 Partial ^{1}H NMR spectra (400 MHz, DMSO-d_6, 298K) of free **G1** + I^- in various concentrations of L-Arg: a) free; b) 1.0; c) 2.0; d) 5.0; e) 10.0 equiv..

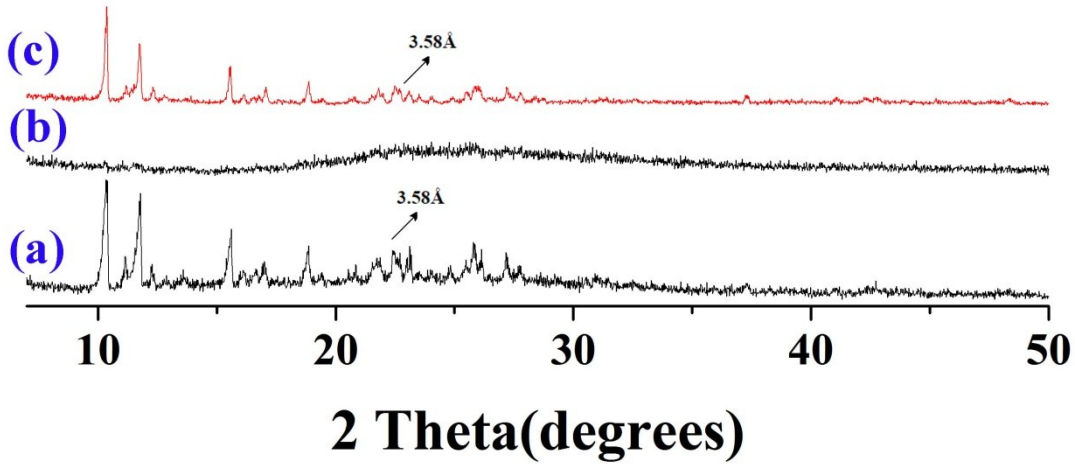


Fig. S9 Powder XRD patterns of (a) ***is*-G**; (b) ***is*-IG;** (c) ***is*-IG** + L-Arg.

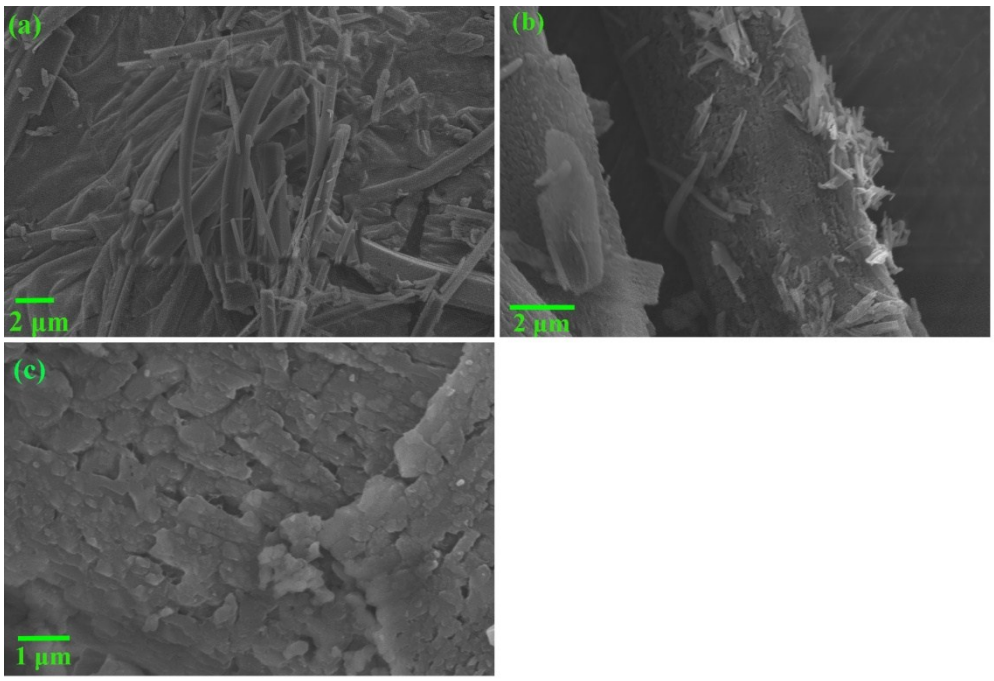


Fig. S10 SEM images of (a) ***is*-FeG**; (b) ***is*-FeG** + L-Ser; (c) ***is*-IG** + L-Arg.

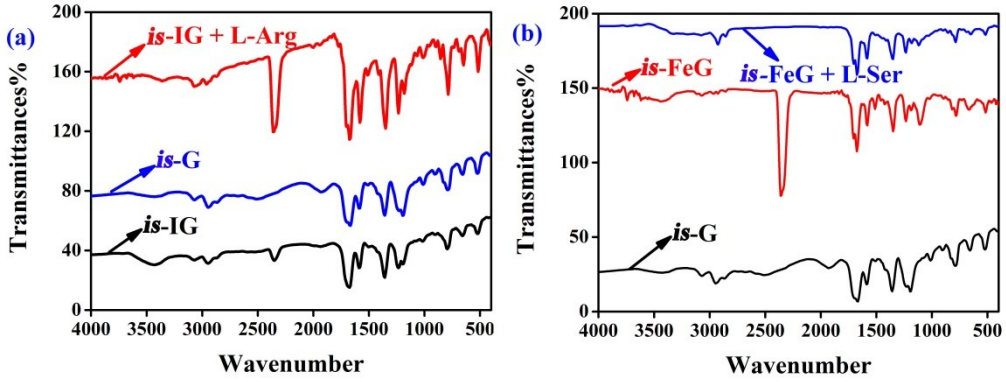


Fig. S11 FT-IR spectra of (a) ***is*-G**, ***is*-IG** and ***is*-IG** + L-Arg; (b) ***is*-G**, ***is*-FeG** and ***is*-FeG** + L-Ser.

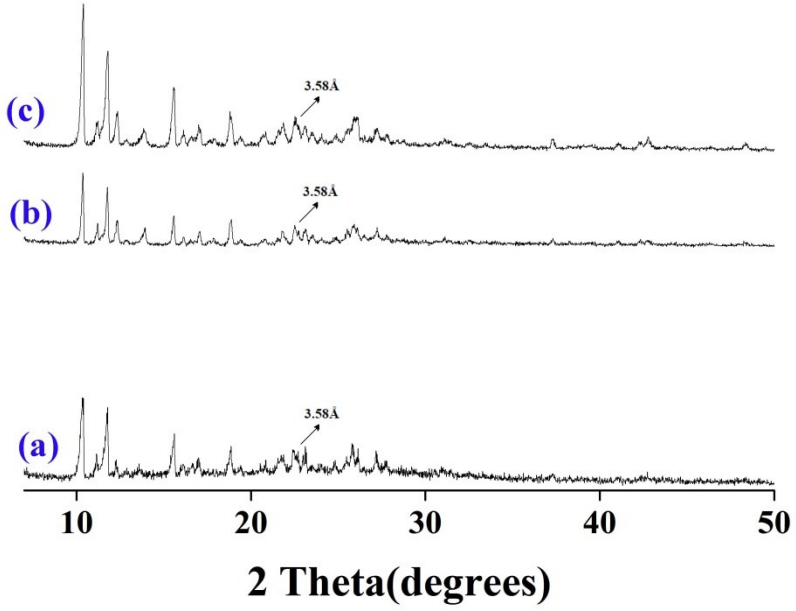


Fig. S12 Powder XRD patterns of (a) ***is*-G**; (b) ***is*-FeG;** (d) ***is*-FeG** + L-Ser.