**Supporting Information for**

# Multicolor emission of nonaromatic linear polysiloxane based on local conjugation chains

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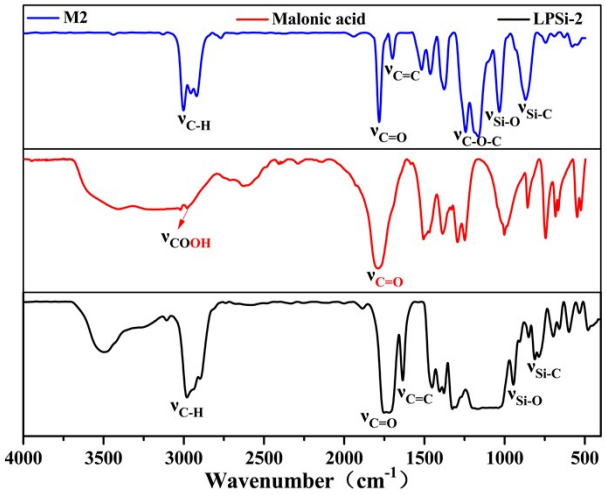


**Fig. S1.** FTIR spectra of LPSi-2, malonic acid, and M2.

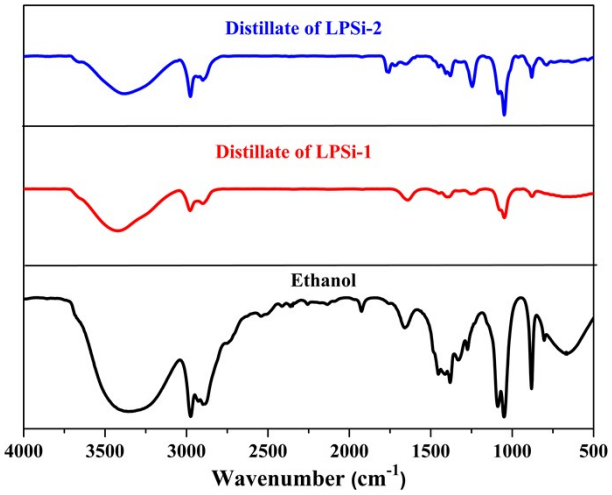


**Fig. S2.** FTIR spectra of distillate of LPSi and standard ethanol.

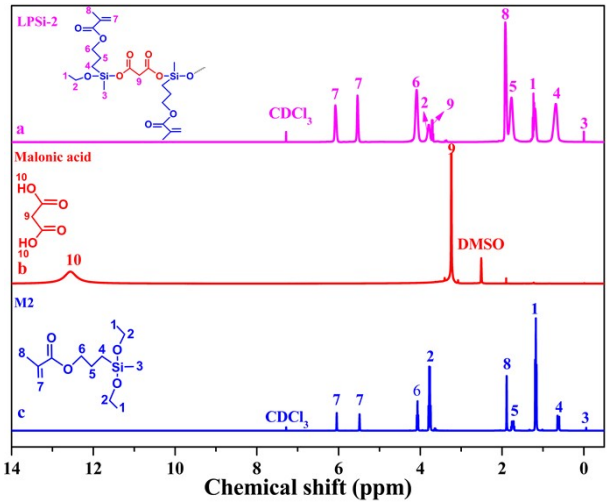


**Fig. S3.** [1]H NMR spectra of LPSi-2, malonic acid and M2.

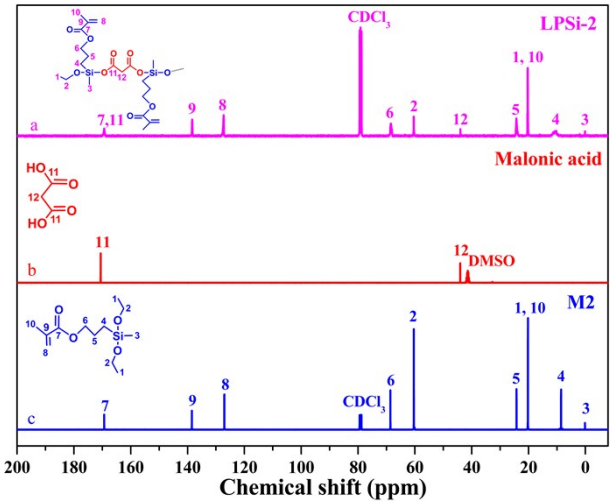


**Fig. S4**. $^{13}C$ NMR spectra of LPSi-2, malonic acid and M2.

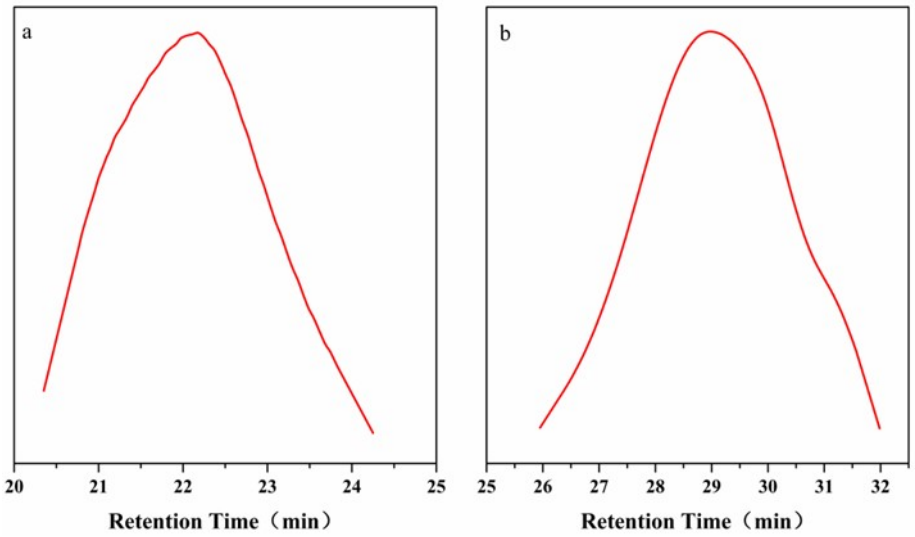


**Fig. S5.** GPC curve of LPSi-1 (a) and LPSi-2 (b).

**Table S1** GPC data of LPSi-1 and LPSi-2.

| Polymer | *Mn* | $M_W$ | $M_Z$ | $M_{Z+1}$ | PDI |
|---|---|---|---|---|---|
| LPSi-1 | 60200 | 70800 | 81800 | 92200 | 1.18 |
| LPSi-2 | 6300 | 6800 | 8500 | 7600 | 1.26 |

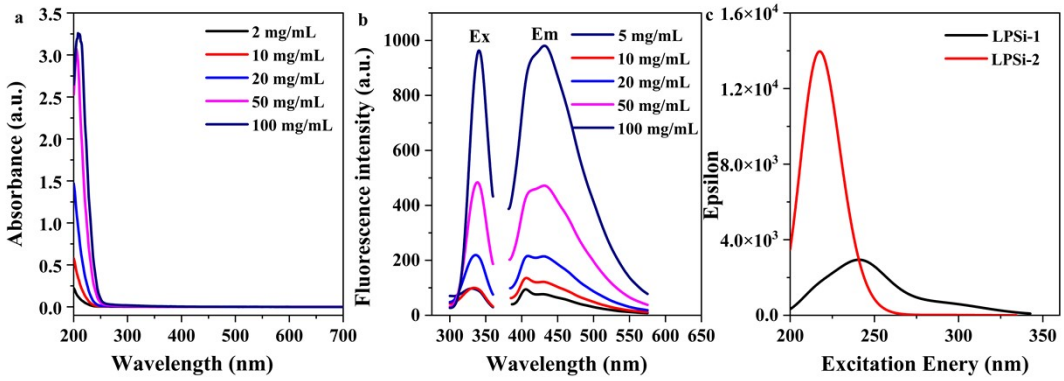


**Fig. S6**. (a) UV–vis absorption spectra and (b) PL spectra of LPSi-2 in the ethanol solution at different concentrations, (c) Theoretical UV-vis spectra for LPSi-1 and LPSi-2 with a degree of polymerization of 3.

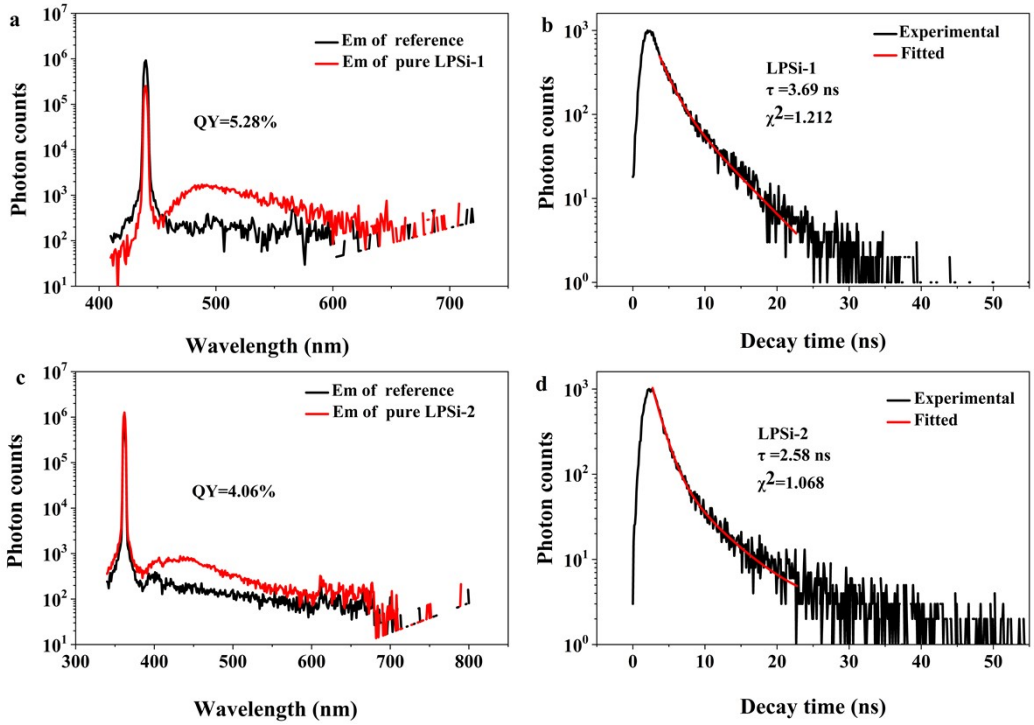


**Fig. S7.** Absolute quantum yield and fluorescence attenuation curve for the pure LPSi-1 (a, b) and LPSi-2 (c, d).

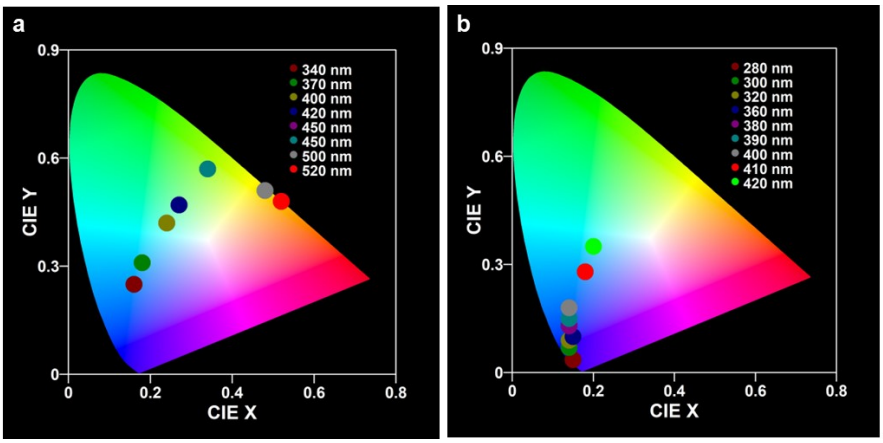


**Fig. S8.** CIE coordinates of LPSi-1 (a) and LPSi-2 (b) in ethanol solution.

**Table S2** The CIE coordinates of LPSi-1 ethanol solution were calculated according to the emission wavelength at different excitation wavelengths.

| Polymer | Excitation | CIE coordinates |
|---|---|---|
| LPSi-1 | 340 nm | (0.16, 0.25) |
| | 370 nm | (0.18, 0.31) |
| | 400 nm | (0.24, 0.42) |
| | 420 nm | (0.27, 0.47) |
| | 450 nm | (0.34, 0.57) |
| | 470 nm | (0.39, 0.58) |
| | 500 nm | (0.48, 0.51) |
| | 520 nm | (0.52, 0.48) |
| LPSi-2 | 320 nm | (0.14, 0.09) |
| | 340 nm | (0.15, 0.09) |
| | 360 nm | (0.15, 0.10) |
| | 380 nm | (0.14, 0.13) |
| | 400 nm | (0.14, 0.18) |
| | 410 nm | (0.18, 0.28) |
| | 420 nm | (0.20, 0.35) |

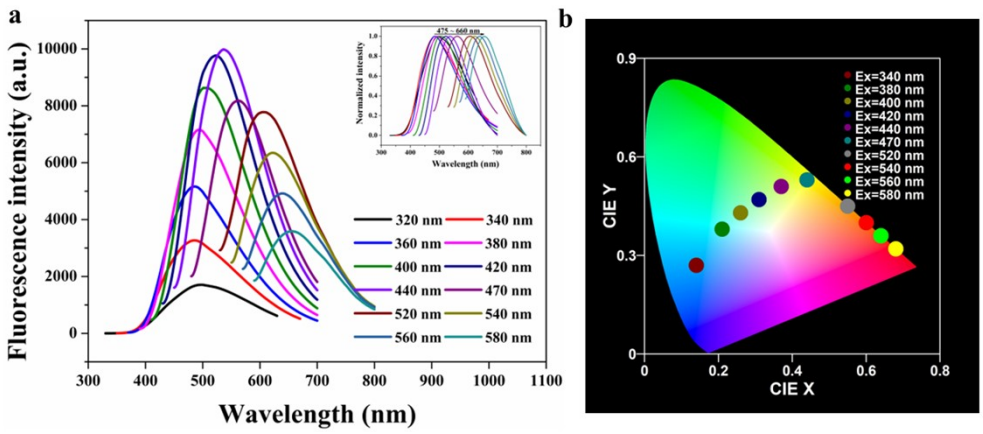


**Fig. S9.** (a) Excitation-dependent photoluminescence of the pure LPSi-1 at varying excitation wavelengths (The inset shows normalized emission); (b) CIE coordinates of pure LPSi-1.

**Table S3** The CIE coordinates of pure LPSi-1 were calculated according to the emission wavelength at different excitation wavelengths.

| Polymer | Excitation | CIE coordinates |
|---|---|---|
| LPSi-1 | 340 nm | (0.14, 0.27) |
| | 380 nm | (0.21, 0.38) |
| | 400 nm | (0.26, 0.43) |
| | 420 nm | (0.31, 0.47) |
| | 440 nm | (0.37, 0.51) |
| | 470 nm | (0.44, 0.53) |
| | 520 nm | (0.55, 0.45) |
| | 540 nm | (0.60, 0.40) |
| | 560 nm | (0.64, 0.36) |
| | 580 nm | (0.68, 0.32) |

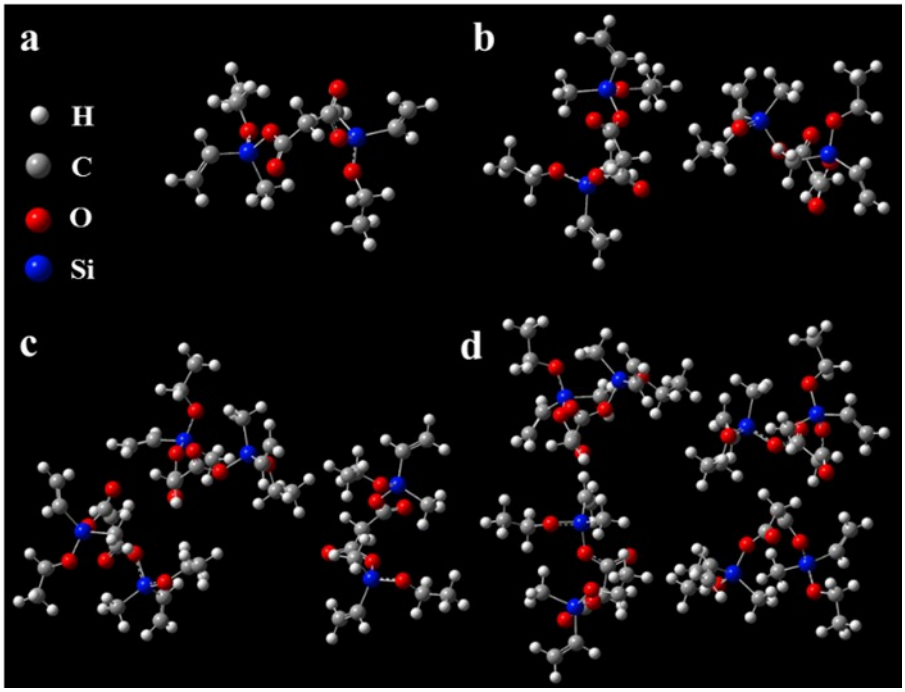


**Fig. S10.** Optimized conformations of aggregation molecules increases from 1 to 4 of LPSi-1 with a degree of polymerization of 1 (a~d).

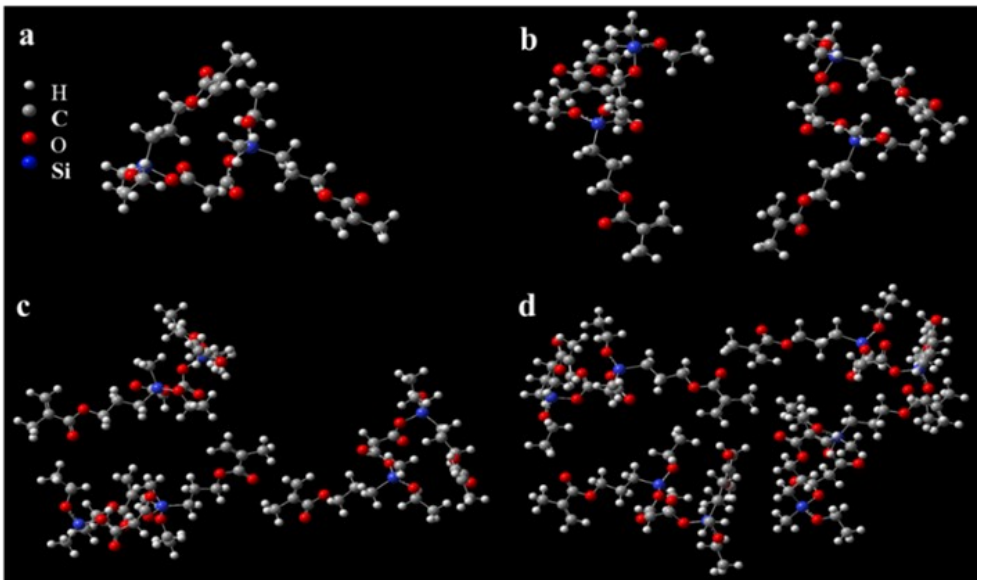


**Fig. S11.** Optimized conformations of aggregation molecules increases from 1 to 4 of LPSi-2 with a degree of polymerization of 1 (a~d).

**Table S4** DFT calculation results of LPSi-1 molecules with polymerization degree 1.

| Molecule number | E(HOMO) a.u | E(LUMO) a.u. | Energy gap/a.u. | Energy gap/eV |
|---|---|---|---|---|
| 1 | -0.264 | -0.015 | 0.249 | 6.764 |
| 2 | -0.263 | -0.017 | 0.246 | 6.695 |
| 3 | -0.260 | -0.017 | 0.243 | 6.604 |
| 4 | -0.260 | -0.019 | 0.241 | 6.564 |

**Tab. S5.** TD-DFT calculation results of oscillator strengths for the LPSi-1 and LPSi-2 with a degree of polymerization of 3.

| Oligomer | LPSi-1 | LPSi-2 |
|---|---|---|
| Excitation energy (nm) | 249.17 | 229.86 |
| Oscillator strengths | 0.0133 | 0.0108 |

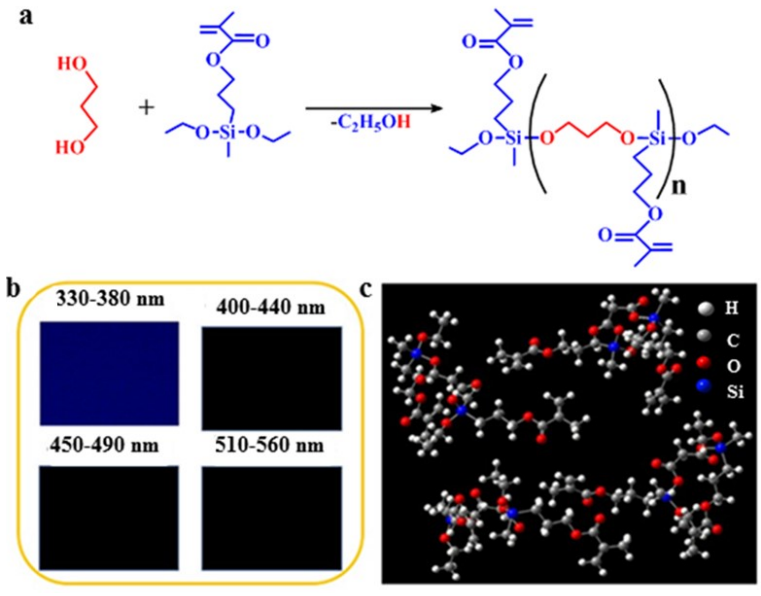


**Fig. S12.** (a) Synthesis route of linear polysiloxane, (b) Fluorescence microscopy images of pure P2 under the light filter of UV-2A (Ex 330−380 nm), BV-2A (Ex 400−440 nm), B-2A (Ex 450−490 nm), and G-2A (Ex 510−560 nm); (c) Optimized conformations of four first generation P2 molecules.[1]

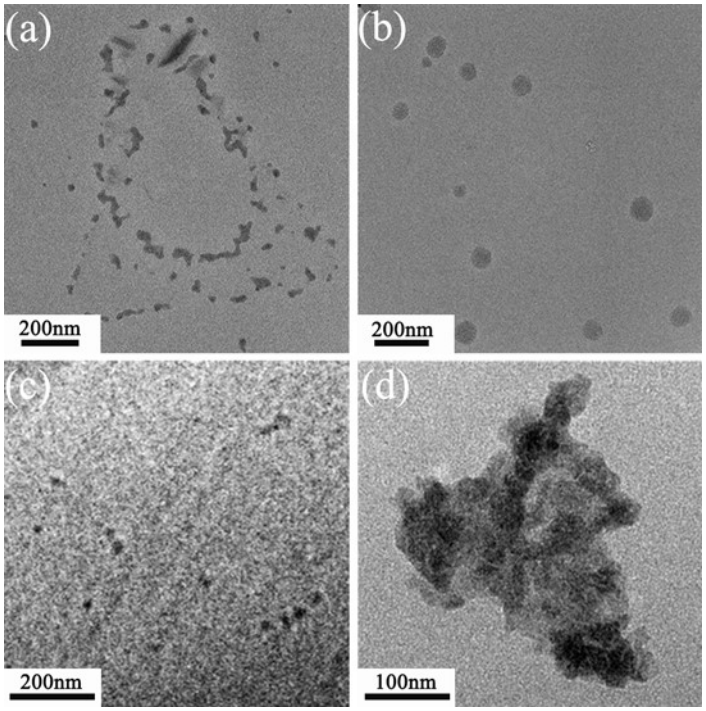


**Fig. S13.** TEM micrographs of self-assembled morphology of LPSi-1 and LPSi-2 in ethanol with the concentration at 10 mg/mL (a, c) and 50 mg/mL (b, d), respectively.

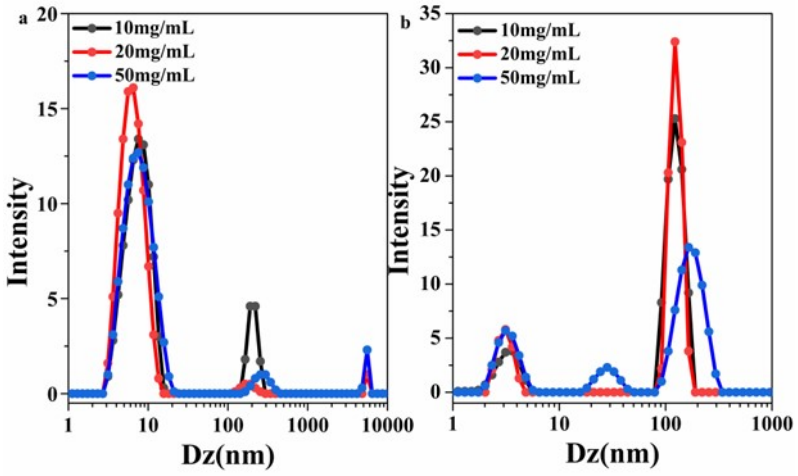


**Fig. S14.** Particle size distribution of LPSi-1 (a) and LPSi-2 (b) ethanol solutions at different concentrations.

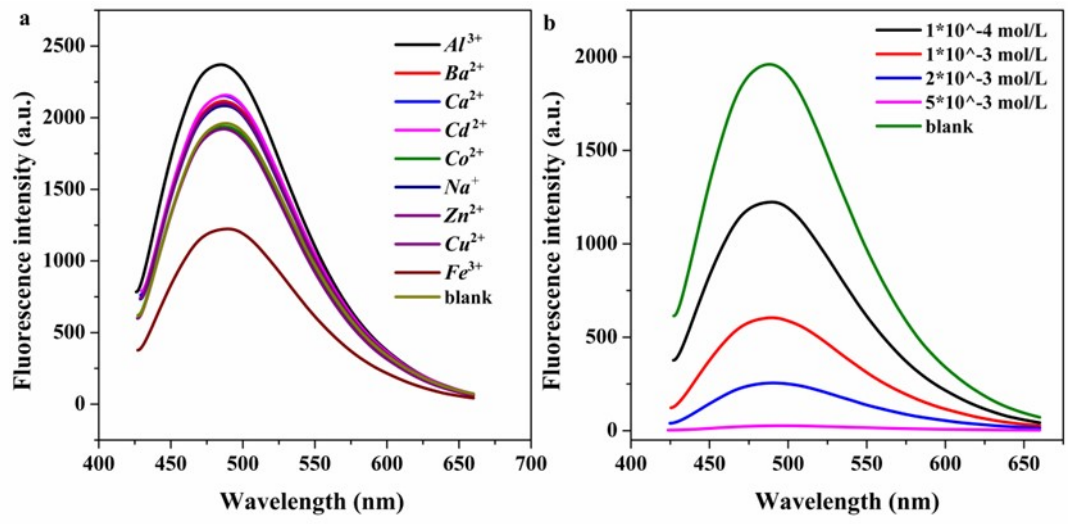


**Fig. S15.** Metal ion sensitivity (a) and effect of the concentration of $Fe^{3+}$ on fluorescence intensity (b) of LPSi-1 at 20 mg/mL ethanol solution.

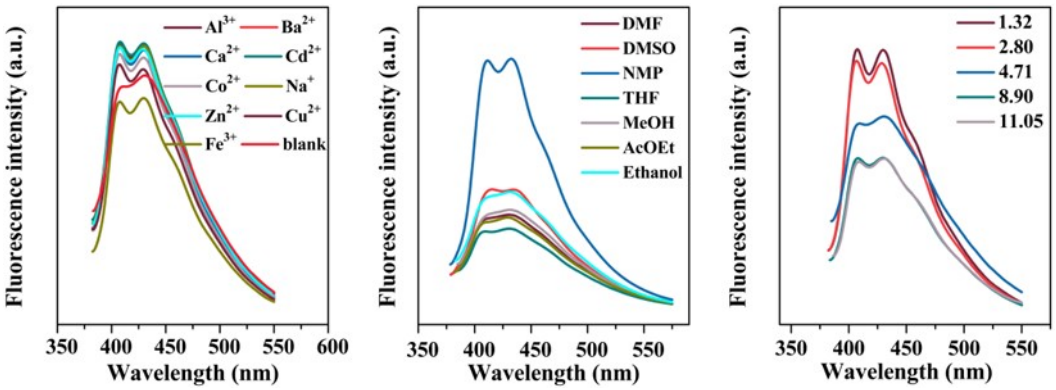


**Fig. S16.** Metal ion sensitivity (a), solvent sensitivity (b) and pH sensitivity (c) of LPSi-2 at 20 mg/mL ethanol solution.

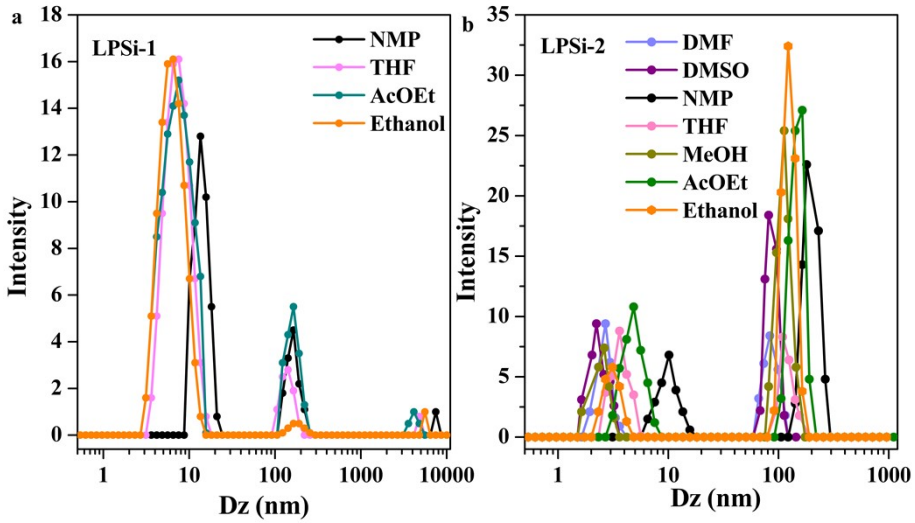


**Fig. S17** The particle size distribution of LPSi-1 and LPSi-2 in different solvents.

## References

1. Y.B. Feng, H.X. Yan, F. Ding, T. Bai, Y. F. Nie, Y. Zhao, W. X. Feng, B. Z. Tang, *Mater. Chem. Front.,* 2020, **4**, 1375-1382.