Formation of lead chalcogenide quantum dot-based supramolecular polymer network via pillar[5]arene-based host-guest complexation

Bingbing Shi,* Yun-Fei Zhang, Zheng-Hua Zhang, Hong Yao, Wen-Juan Qu, You-Ming Zhang, Tai-Bao Wei, Qi Lin*

Key Laboratory of Eco-Functional Polymer Materials of the Ministry of Education, College of Chemistry and Chemical Engineering, Northwest Normal University, Lanzhou 730070, P. R. China E-mail: bingbingshi@nwnu.edu.cn; linqi2004@126.com

Supporting Information (13 pages)

1.	Synthesis of 1 and 2	S2
2.	Host-guest complexation study	S 8
3.	2D DOSY NMR experiments	S10
4.	Dynamic light scattering study	S11
5.	Metal-ligand coordination study	S12
6.	Visual fluorescence emission photos	S13
7.	Controlled experiments	S13

















Figure S8. ¹H NMR spectrum (400 MHz, CDCl₃, 298 K) of **1**.



Figure S10. High-resolution mass spectrum of 1.





Figure S13. High-resolution mass spectrum of 2.

2. Host–guest complexation study



Figure S14. Partial ¹H NMR (400 Hz, DMSO-*d*₆, 298 K) spectra: (a) guest molecule **2** (1.50 mM); (b) **1** (1.00 mM) and **2** (1.50 mM); (c) host **1** (1.00 mM).



Figure S15. Partial 2D NOESY NMR (600 MHz, DMSO- d_6 , 298 K) spectrum of a solution of 1 (1.00 mM) and 2 (1.50 mM).



Figure S16. Partial 2D NOESY NMR (600 MHz, DMSO-*d*₆, 298 K) spectrum of a solution of **1** (1.00 mM) and **2** (1.50 mM).

3. 2D DOSY NMR experiments



Figure S18. 2D DOESY NMR (500 MHz, DMSO-d₆, 298 K) spectrum of 2 (1.50 mM).



Figure S19. 2D DOESY NMR (500 MHz, DMSO-*d*₆, 298 K) spectrum of **1** (1.00 mM) + **2** (1.50 mM).

4. Dynamic light scattering study



Figure 20. Correlation coefficient in DLS result of the assemblies of 1 and 2 complex in DMSO/H₂O (v : v = 4 : 1).

5. Metal-ligand coordination study



Figure S21. ¹H NMR spectra (400 MHz, DMSO- d_6) of **1** (1.00 mM) in the presence of different concentrations of Pb²⁺ ions. (a) 0 mM; (b) 0.500 mM.; (c) 1.00 mM; (d) 1.50 mM; (e) 2.00 mM; (f) 3.00 mM.



Figure S22. ¹H NMR spectra (400 MHz, DMSO- d_6) of (a) **1** (1.00 mM) and (b) in the presence of 5.00 equivalents of HCl.

The intermolecular and intramolecular hydrogen bonds of monomer 1 were investigated by the ¹H NMR experiment. As shown in Figure S22, after the addition of 5.00 equivalents of HCl to the solution of 1 (1.00 mM), the peaks related to the protons H_1 and H_2 of monomer 1 showed up-field shifts, indicating the break of the intermolecular and intramolecular hydrogen bonds of monomer 1.

6. Visual fluorescence emission photos



Figure S23. Visual fluorescence emission of (A) supramolecular polymer network containing Pb²⁺ ions and the Pb²⁺ containing supramolecular polymer network upon the addition of (B) F⁻, (C) Cl⁻, (D) Br⁻,(E) I⁻, (F) AcO⁻, (G) H₂PO₄⁻, (H) HSO₄⁻, (I) ClO₄⁻, (J) CN⁻ and (K) S²⁻ (10.0 mM), respectively in DMSO/H₂O (v : v = 4 : 1) under excitation at 365 nm using a UV lamp at rt.

7. Controlled experiments



Figure S24. (a) SEM image of the complex of **1** (1.00 mM) + Pb²⁺ (3.00 mM) + S²⁻ (10.0 mM) in DMSO/H₂O (v : v = 4 : 1). (b) SEM image of the complex of **2** (1.50 mM) + Pb²⁺ (3.00 mM) + S²⁻ (10.0 mM) in DMSO/H₂O (v : v = 4 : 1).