

Electronic Supplementary information for

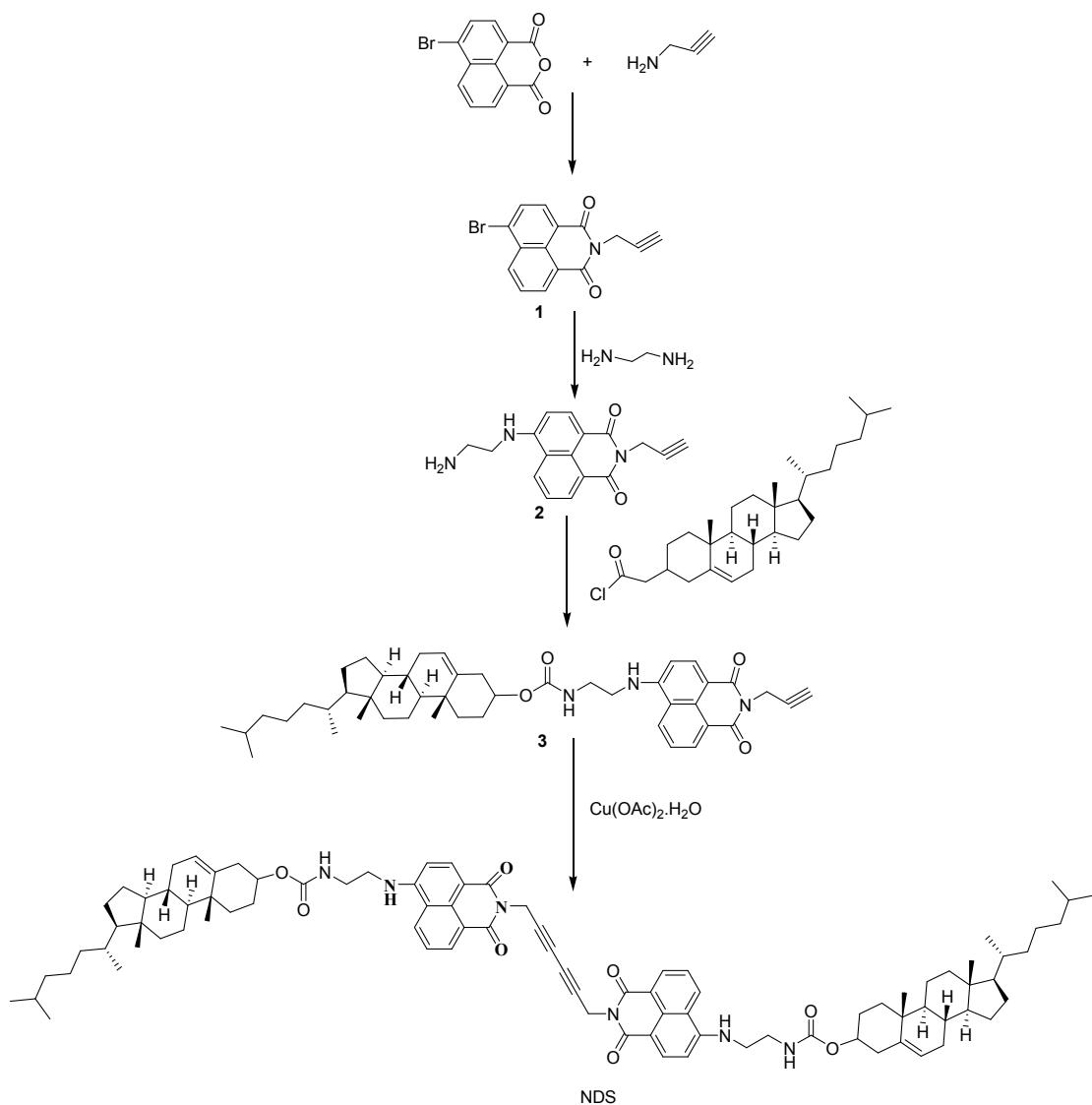
**Effect of water on the supramolecular assembly and  
functionality of naphthalimide derivative: tunable  
honeycomb structure with mechano-chromic properties**

Xudong Yu,<sup>a\*</sup> Dongyan Xie,<sup>a</sup> Haichuang Lan,<sup>b</sup> Yajuan Li,<sup>a</sup> Xiaoli Zhen,<sup>a</sup> Jujie Ren,<sup>a</sup> Tao Yi,<sup>b\*</sup>

<sup>a</sup>College of Science and Hebei Research Center of Pharmaceutical and Chemical Engineering, Hebei University of Science and Technology, Yuhua Road 70, Shijiazhuang 050080, PR China

<sup>b</sup>Department of Chemistry and Collaborative Innovation Center of Chemistry for Energy Materials, Fudan University, 220 Handan Road, Shanghai 200433, China

\*E-mail for corresponding author: [081022009@fudan.edu.cn](mailto:081022009@fudan.edu.cn) (X. D. Yu),  
[yitao@fudan.edu.cn](mailto:yitao@fudan.edu.cn) (T. Yi)



Scheme S1 the synthesis procedure of **NDS**.

The synthesis of compounds **1-3** could be seen in our previous report.<sup>37</sup>

**Synthesis of NDS:** compound 3 (567 mg, 0.8 mmol),  $\text{Cu}(\text{OAc})_2$  (161 mg, 0.8 mmol) were heated in pyridine at 60°C for 10 h, then the reaction mixture was concentrated and purified by column chromatography ( $\text{SiO}_2$ ,  $\text{CH}_2\text{Cl}_2$ :  $\text{CH}_3\text{OH}$ =200:1), resulting in yellow solid (227 mg, yield: 40%) M.p. 133-135 °C.  $^1\text{H}$ NMR (500 M,  $\text{DMSO}-d_6$ ,  $\delta$ ): 0.68 (s, 6H), 0.86-0.87 (d,  $J=2$  Hz, 6H), 0.88 (d,  $J=2$  Hz, 6H), 0.92-0.93 (d,  $J=8$  Hz, 6H), 1.0-2.36 (m, 62H), 3.38-3.39 (t,  $J=6$  Hz, 4H), 3.61-3.64(t,  $J=6$  Hz, 4H), 4.55-5.57

(m, 2H), 4.94 (s, 4H), 5.57-5.39 (m, 2H), 6.33-6.36 (d, J=11 Hz, 2H), 7.34-7.39 (t, J= 10.5Hz, 2H), 7.97-7.99 (d, J=11 Hz, 2H), 8.16-8.18(d, J=10.5 Hz, 2H), 8.24-8.26 (d, J=10.5 Hz, 2H).<sup>13</sup>CNMR (125M, DMF-*d*<sub>6</sub>,*δ*): 11.83, 14.13, 18.63, 19.27, 21.01, 22.51, 22.76, 23.79, 24.58, 26.70, 27.97, 28.18, 29.64, 30.15, 31.38, 31.87, 33.23, 35.80, 36.15, 36.68, 37.45, 38.78, 39.48, 39.70, 50.18, 56.12, 58.74, 103.25, 119.07, 122.80, 123.92, 124.41.  
MALDITOF        calc.        for        [C<sub>90</sub>H<sub>116</sub>N<sub>6</sub>O<sub>8</sub>+K]<sup>+</sup>,        1447.8492;  
[C<sub>90</sub>H<sub>115</sub>N<sub>6</sub>O<sub>8</sub>+H]<sup>+</sup>:1409.8933; Found: 1447.8171, 1409.8837.

Table S1 the gelation properties of **NDS** (25 mg/mL) in different organic solvents.

Solvent	H-C	U
CHCl <sub>3</sub>	G	S
n-butanol	P	G
CH <sub>2</sub> Cl <sub>2</sub>	G	S
DMF	S	S
n-propanol	S	S
ethyl acetate	P	P
acetone	P	P
THF	S	S
glycol monomethyl ehter	I	I
methanol	I	I

Note: G: gel; S: solution; P: precipitate; I: insoluble; H-C: heating-cooling process; U: ultrasound.

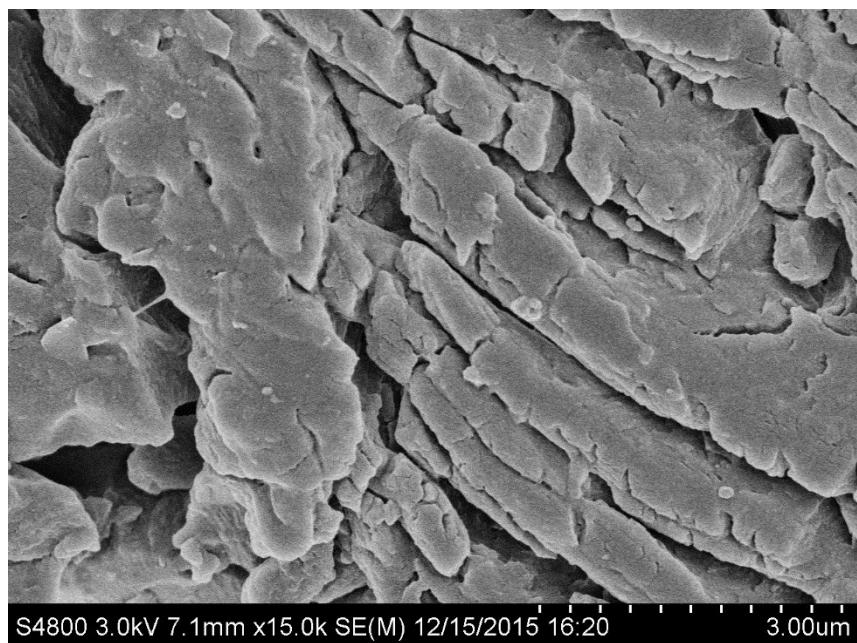


Fig. S1 The SEM image of powder of **NDS** from column chromatography.

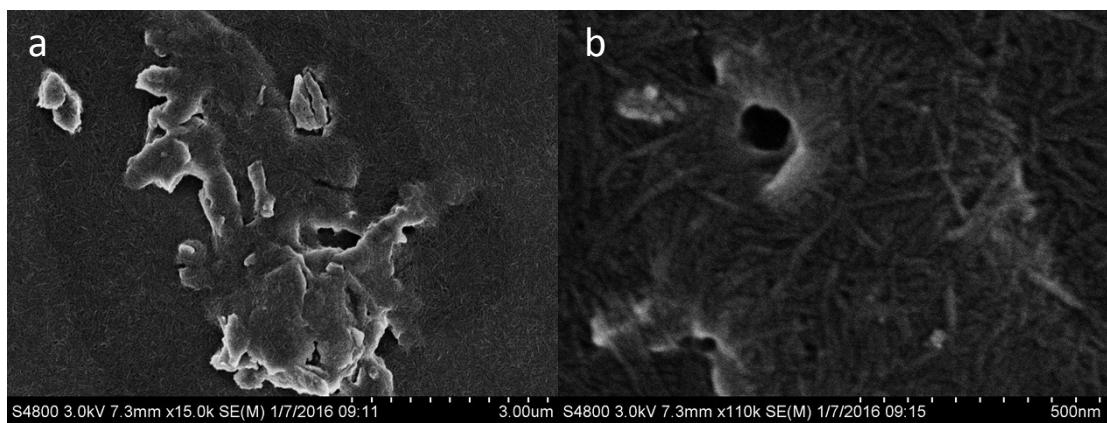


Fig. S2 a) the SEM image of xerogel of **NDS** from  $\text{CHCl}_3$  (25 mg/mL) by centrifugation method; b) the magnification picture of a).

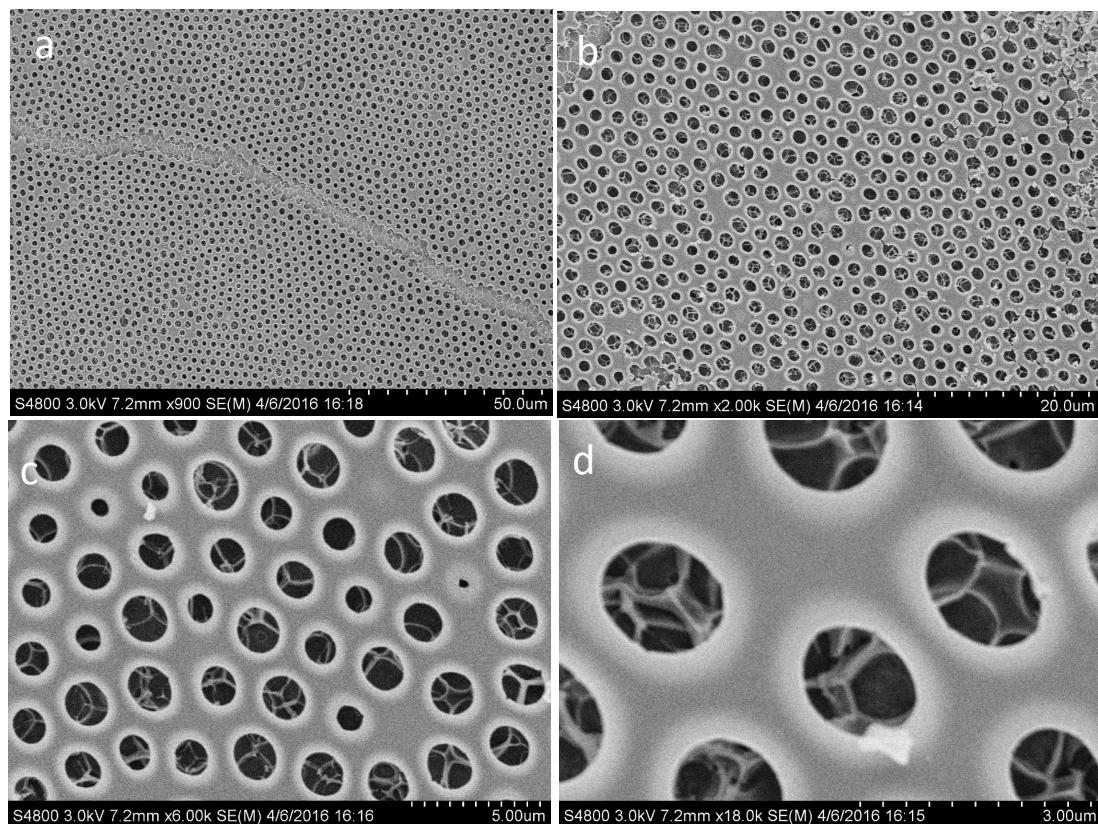


Fig. S3 Large scale, multilayer honeycomb structure of **NDS** xerogel (25 mg/mL) from  $\text{CHCl}_3$  by shaking-rest method.

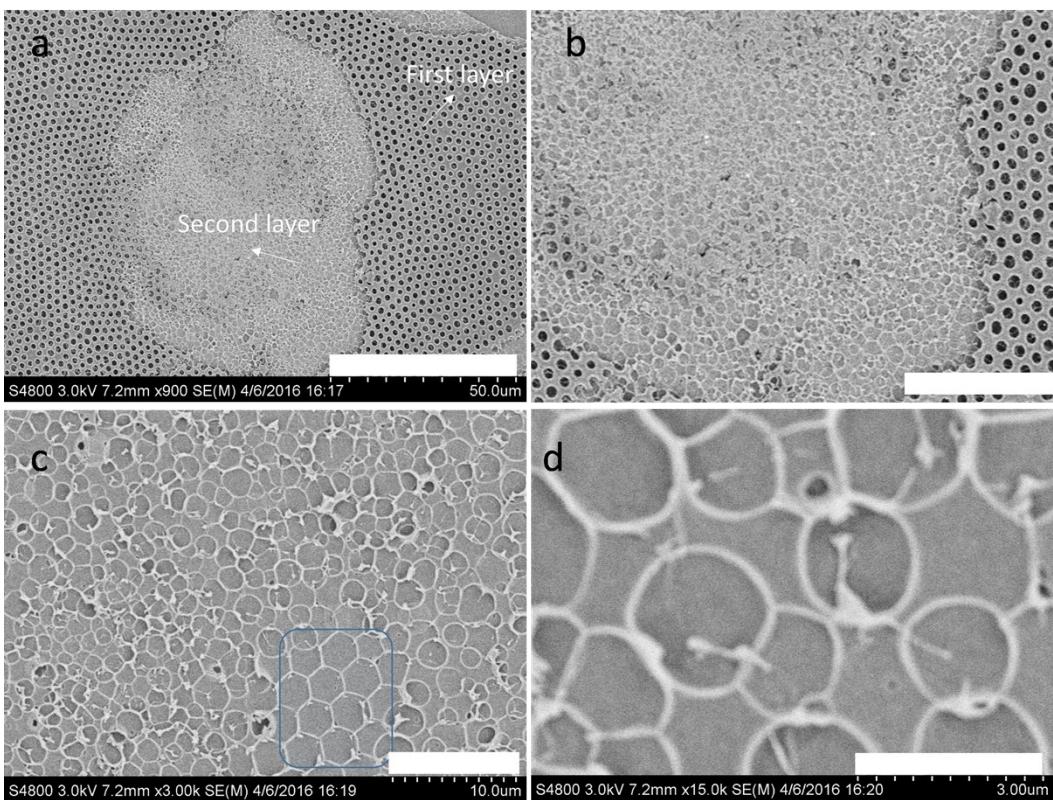


Fig. S4 SEM images of boundaries of the honeycomb structure with second layer.

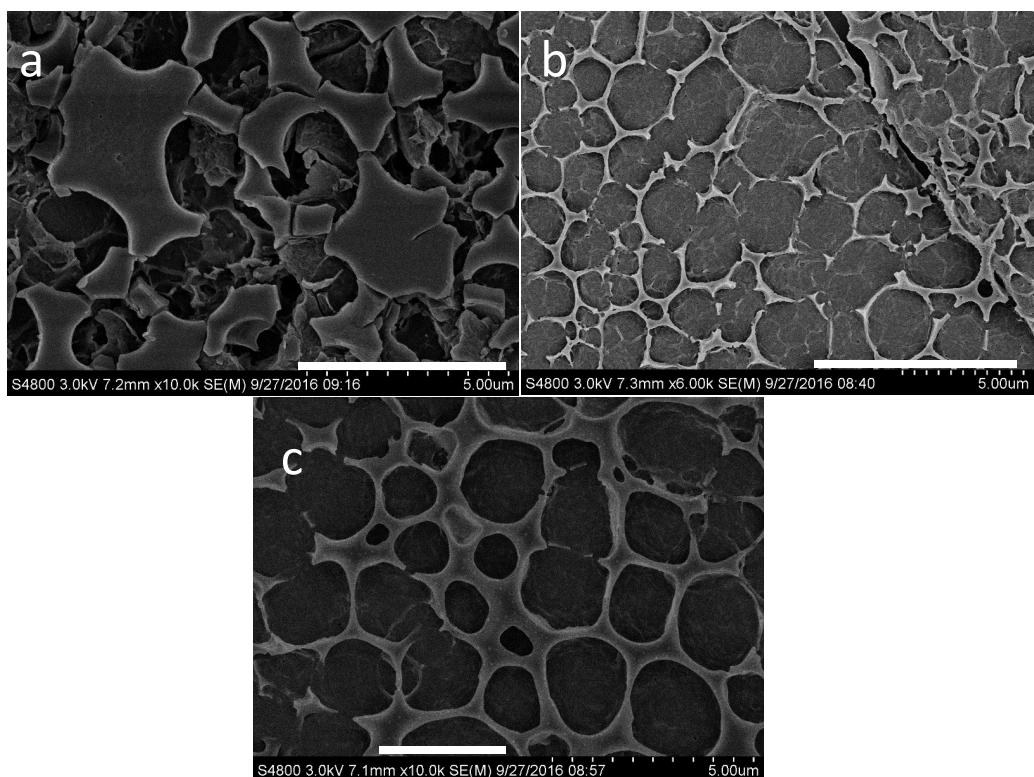


Fig. S5 SEM images of NDS aggregates by evaporation method. a) 7

mg/mL; b) 9 mg/mL; c) 12.5 mg/mL. Scale bar: a) 5  $\mu$ m; b) 5  $\mu$ m; c) 5  $\mu$ m.

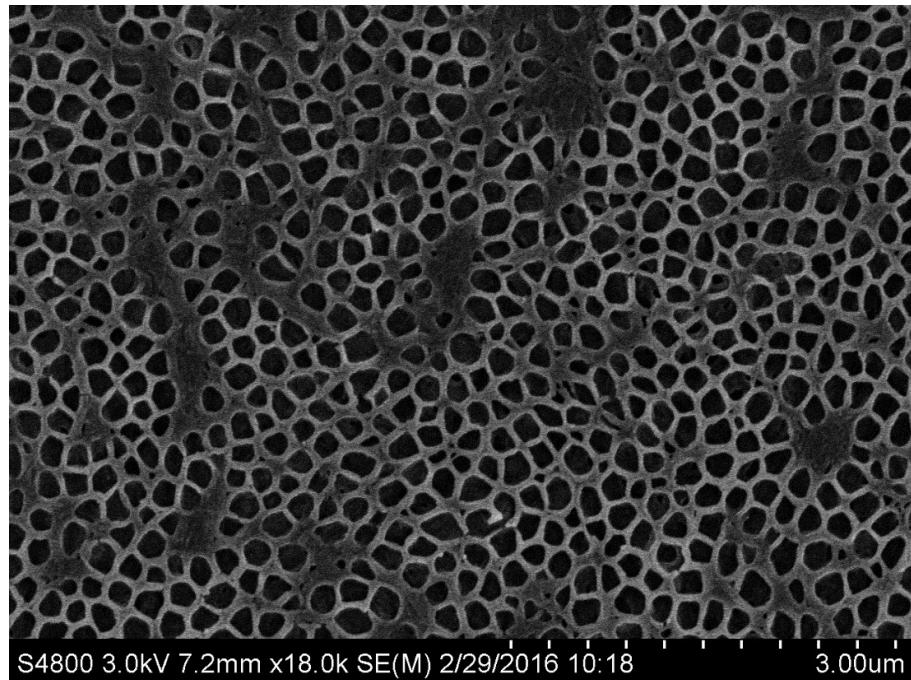


Fig. S6 SEM image of xerogel from gel emulsion **NDS** containing 50% water (25 mg/mL).

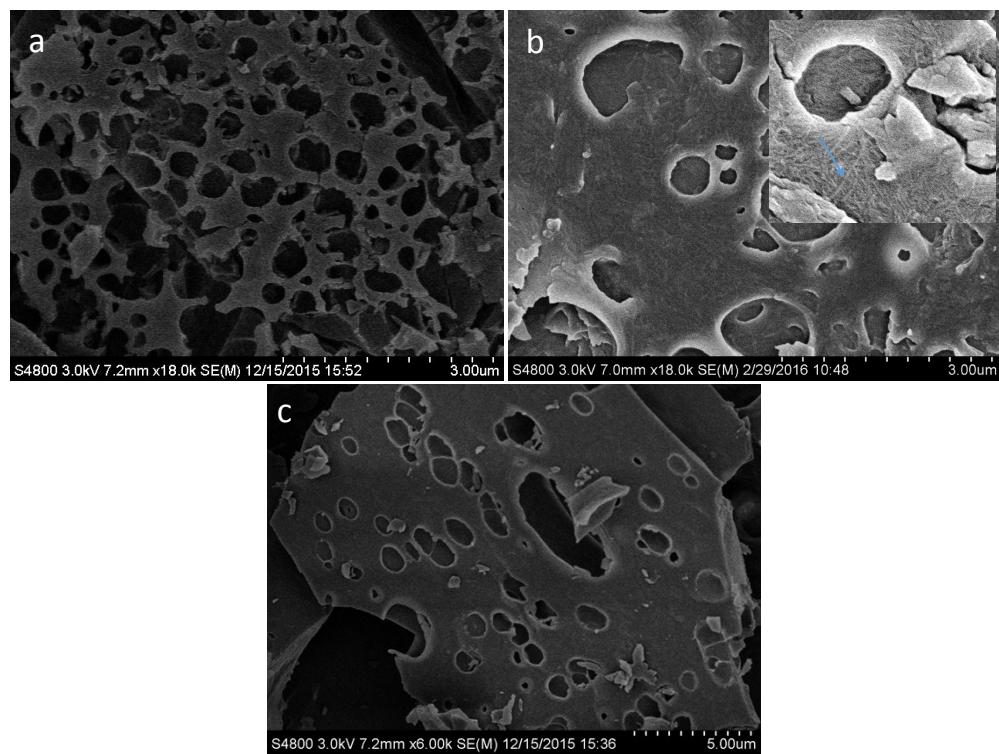


Fig. S7 SEM images of the **NDS** xerogels from gel emulsions. a) gel emulsion containing 60% water; b) gel emulsion containing 80% water; c) gel emulsion containing 90% water.

gel emulsion containing 92.5% water.

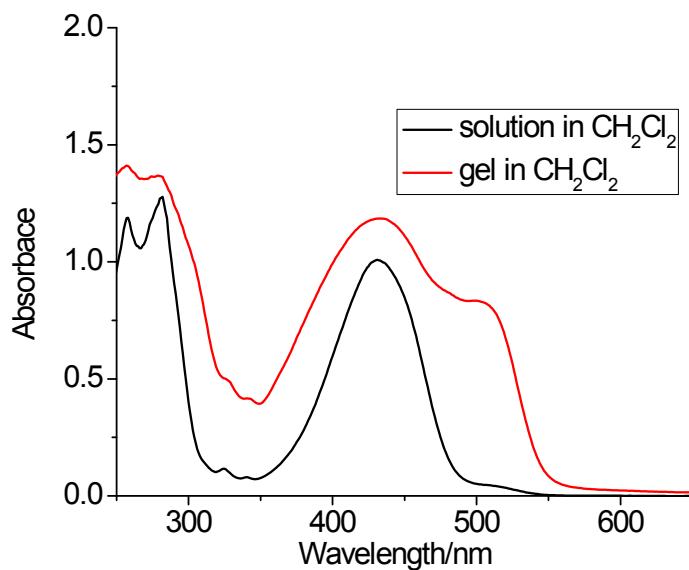


Fig. S8 UV-vis spectra of **NDS** solution ( $10^{-4}$  M) and gel in  $\text{CH}_2\text{Cl}_2$  (25 mg/mL).

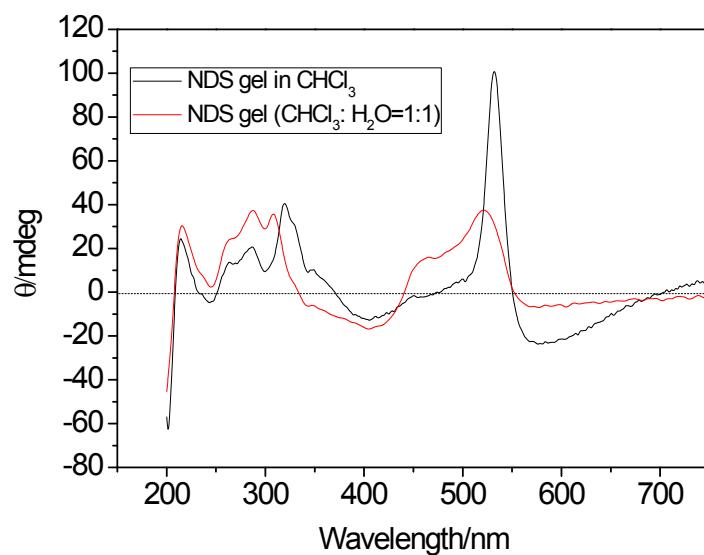


Fig. S9 CD data of **NDS** gels (25 mg/mL).

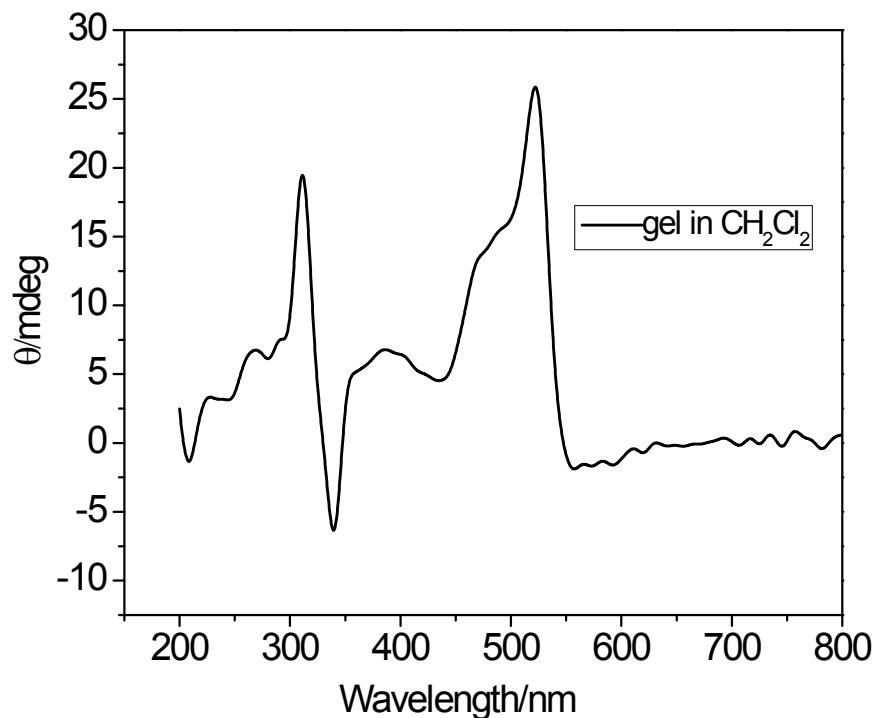


Fig. S10 CD spectra of **NDS** gel in  $\text{CH}_2\text{Cl}_2$ .

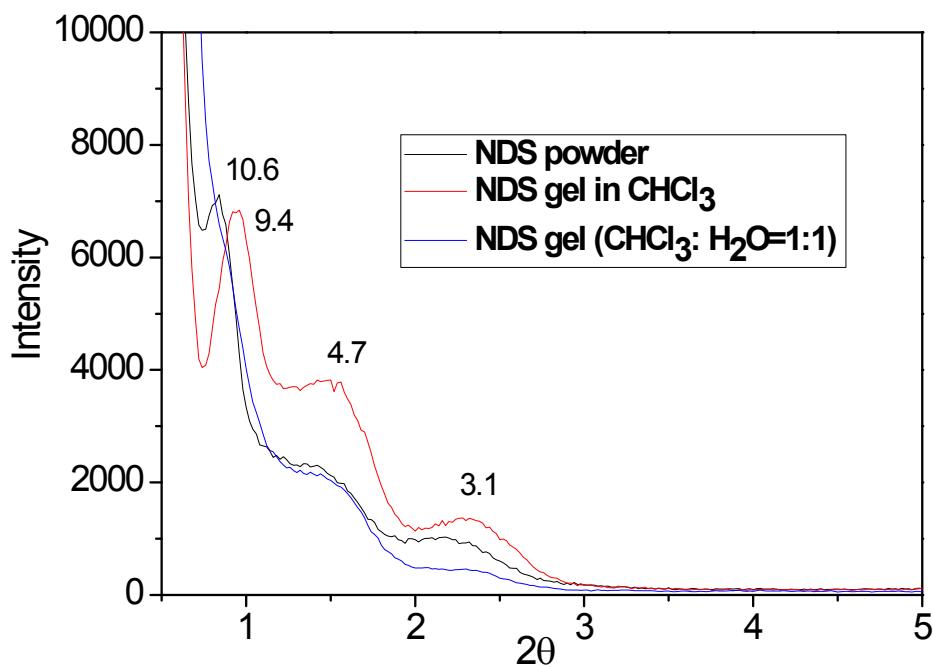


Fig. S11 XRD data of the powder, xerogel from  $\text{CHCl}_3$  and xerogels from gel emulsions of **NDS**.

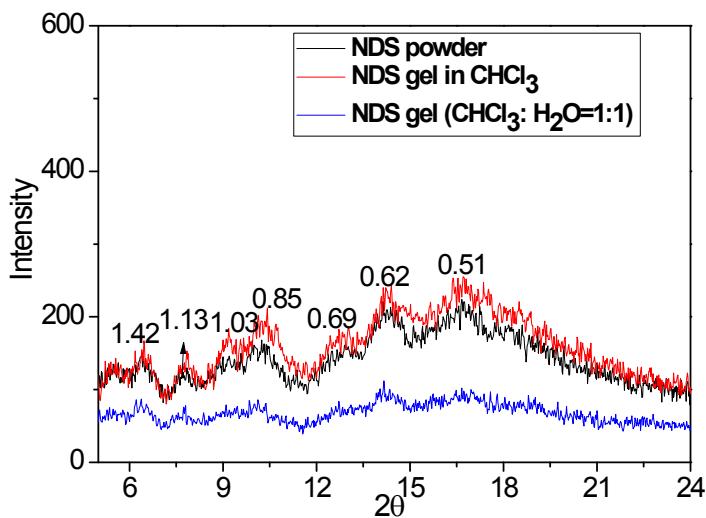


Fig. S12 XRD data of the powder, xerogel from  $\text{CHCl}_3$  and xerogels from gel emulsions of **NDS**.

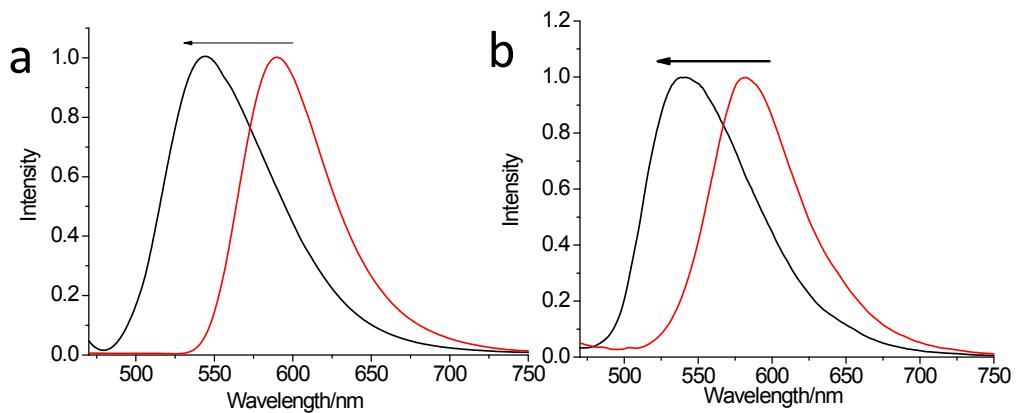


Fig. S13 The fluorescent spectral changes of xerogels from gel emulsions ( $\lambda_{\text{ex}}=450$  nm). a) gel emulsion containing 50% water (from 588 to 543 nm); b) gel emulsion containing 63% water (from 582 to 540 nm).

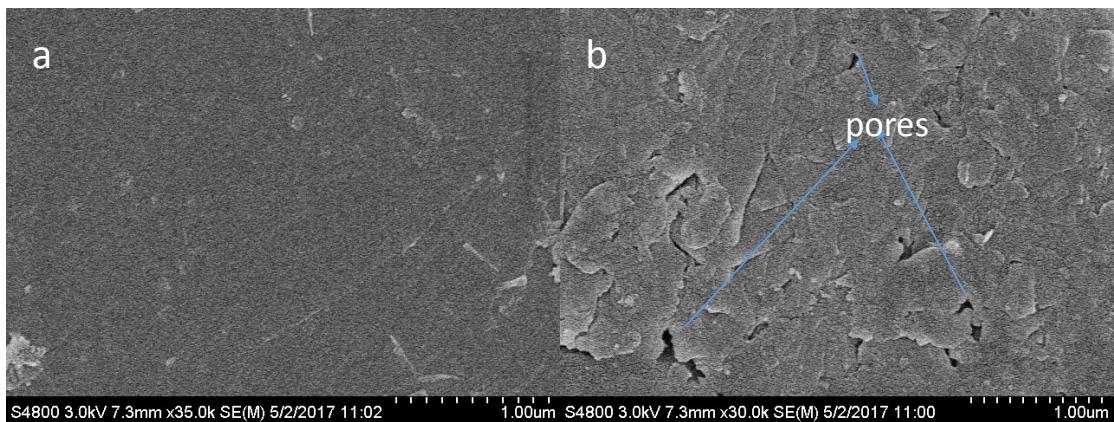


Fig. S14 a) SEM images of NDS xerogel obtained from  $\text{CHCl}_3$  after grinding; b) other area of the xerogel after grinding.

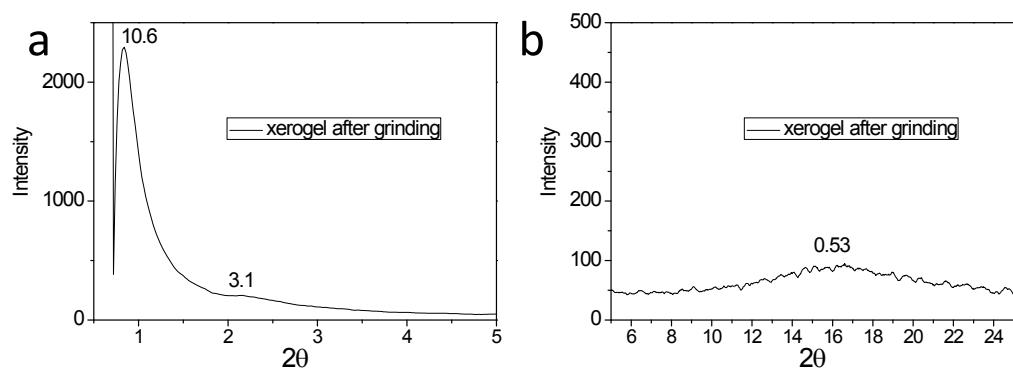


Fig. S15 XRD data of the xerogel from  $\text{CHCl}_3$  after grinding. a)  $0.5^\circ$ - $5^\circ$ ; b)  $5^\circ$ - $25^\circ$ .