Electronic Supplementary Material (ESI) for Soft Matter.

DNA liquid crystals with AIE effect toward humidity-indicating biomaterials

Guoqiang Zhang,[a] Jing Zhao,[b] Qikai Liang,[a] Zhongtao Wu,*[a] Lei Zhang,*[a] Xiliang Luo*[a]

[a]Key Laboratory of Optic-electric Sensing and Analytical Chemistry for Life Science, MOE; Shandong Key Laboratory of Biochemical Analysis; College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao, 266042, China.
[b]Beijing Institute of Big Data Research, Beijing, China.

E-mail: wuzhongtao@qust.edu.cn, zhanglei@qust.edu.cn, xiliangluo@qust.edu.cn

1. General remarks

Materials: Didodecyldimethylammoniumbromide (DDAB), cetyltrimethylammonium bromide (CTAB), sodium dodecylsulfate (SDS) and all the starting materials for synthesizing TPEA were purchased and used without further purification. Single stranded DNA (5'-CCTCGCTCTGCTAATCC TGTTA-3', M.W. = 6612.4) purchased from Sangon Biotech (Shanghai). TPEA was synthesized by following a reported procedure from us, and the chemical structure was confirmed by NMR.[1]

Characterizations: DSC was performed by a Netzsch DSC204F1 machine with a heating/cooling rate of 5^{o}C min^{-1}. TGA was carried out using a Netzsch STA 449C thermal analyzer in a nitrogen atmosphere and with a heating/cooling rate of 10 ^{o}C min^{-1}. POM was conducted on a Nikon ECLIPSE LV100NPOL machine with a computational controlled heating plate. SAXS was performed by employing a conventional X-ray source with radiation wavelength of λ= 1.54 Å. The sample holder is a metal plate with a small hole (diameter ≈ 0.5 cm, thickness ≈ 0.5 cm), where the X-ray beam passes through, and the sample-to-detector distance was 20 cm. The scattering vector q is defined as $q = 4\pi \sin\theta/\lambda$ with 2θ being the scattering angle. Fluorescence spectra were recorded by using a F-4600 fluorescence spectrophotometer from Hitachi, Japan. All spectral scans were saved as ACS II files and further processed in OriginLab software to produce all graphs shown.

2. Syntheses of DNA LCs

DNA-DDAB and DNA-CTAB: to an aqueous solution of DDAB (25 mM, 132 μL) or CTAB (25 mM, 132 μL) was added the aqueous solution of DNA (3.1 mM, 10.10 μL) using a pipette, which led to the precipitate. The precipitate was collected by centrifugation with rcf of 6124 g in an H1-16KR Centrifuge from Hunan Kechengyiqi Co., Ltd, China. The obtained precipitate was washed with water and centrifuged over three times. The resulted wet precipitate was pretreated with liquid nitrogen and then put into a SCIENTZ-10N Lyophilizer from Ningbo Scientz Biotechnology Co, Ltd, China for a lyophilization with -80^{o}C overnight, affording the needed of DNA-DDAB or DNA-CTAB complex.

DNA-DDAB@SDS and DNA-DDAB@TPEA: to an aqueous solution (132 μL) of DDAB (25 mM) and

SDS (0.5 μM for 2%, 1.0 μM for 4%, 1.5 μM for 6%, 2.0 μM for 8%) or TPEA (0.25 μM for 1%, 0.75 μM for 3%, 1.25 μM for 5%) was added the aqueous solution of DNA (3.1 mM, 10.10 μL) using a pipette, which led to the precipitate. The precipitate was collected by centrifugation with rcf of 6124 g in an H1-16KR Centrifuge from Hunan Kechengyiqi Co., Ltd, China. The obtained precipitate was washed with water and centrifuged over three times. The resulted wet precipitate was pretreated with liquid nitrogen and then put into a SCIENTZ-10N Lyophilizer from Ningbo Scientz Biotechnology Co, Ltd, China for a lyophilization with -80^{o}C overnight, affording the needed of DNA-DDAB@SDS and DNA-DDAB@TPEA complexes.

3. Characterizations of DNA LCs

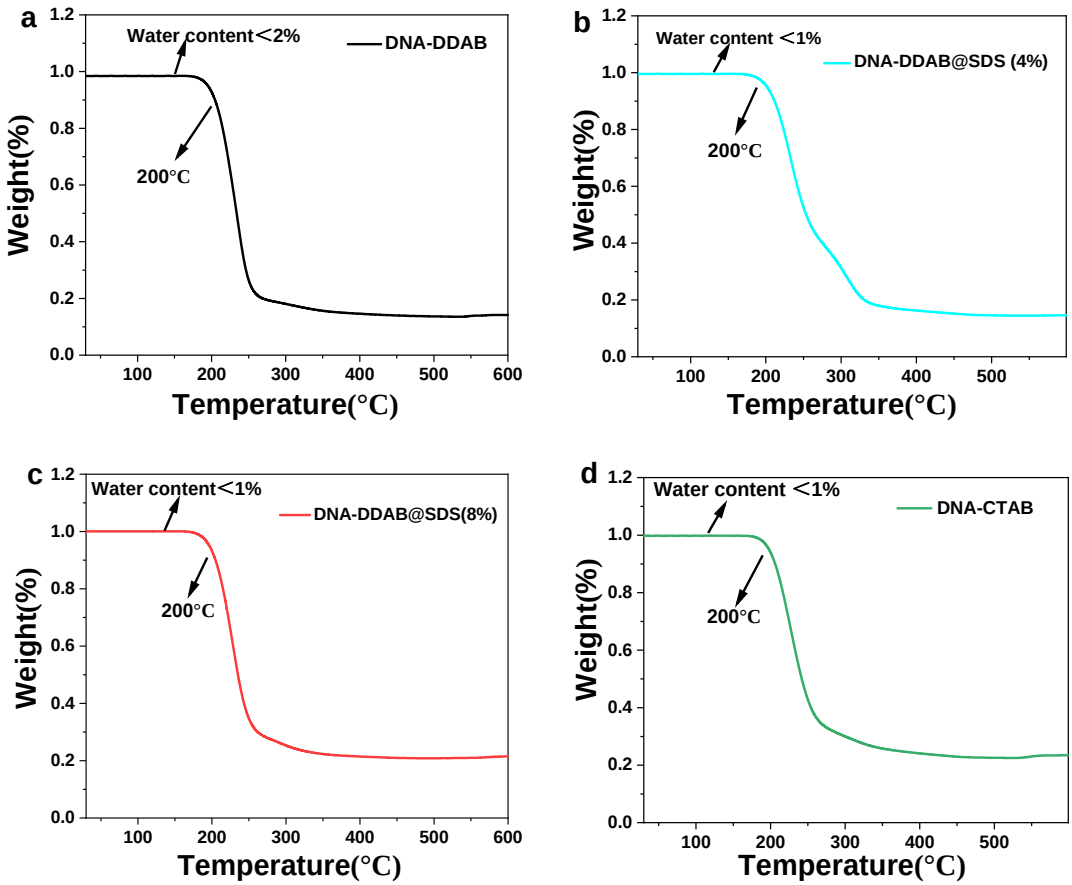

Figure S1. TGA profiles of a) DNA-DDAB, b) DNA-DDAB@SDS (4%), c) DNA-DDAB@SDS (8%) and d) DNA-CTAB. Heating rate: 10 °C min^{-1}.

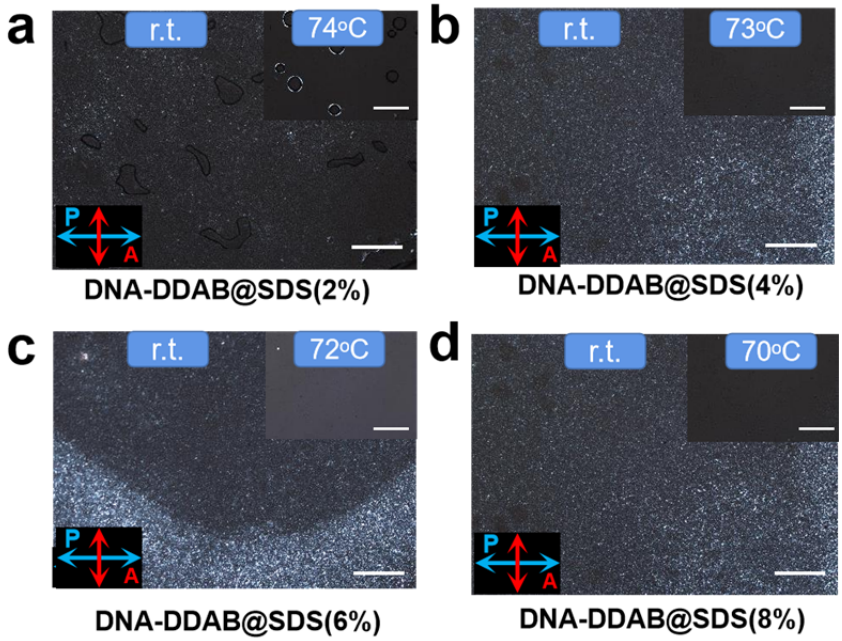

Figure S2. Temperature-dependent POM analyses for determining the T_c of DNA-DDAB@SDS LCs. Scale bar: 20 µm.

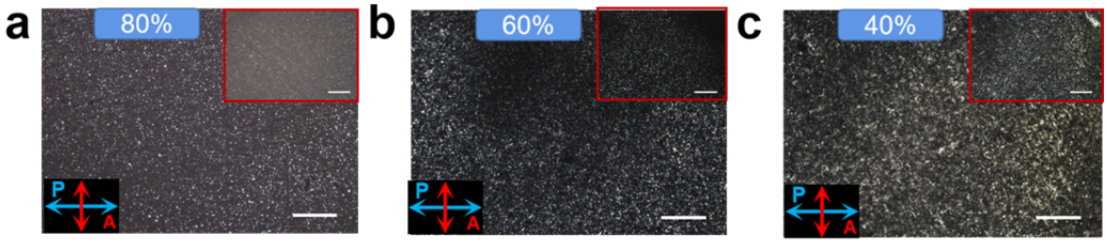

Figure S3. POM analyses on the humidity-induced phase changes of DNA-DDAB under a) RH = 80%, b) RH = 60% and c) RH = 40% with 1 h incubation time at r.t. Scale bar: 20 µm. Upper right insets: the physical states after 1 h.

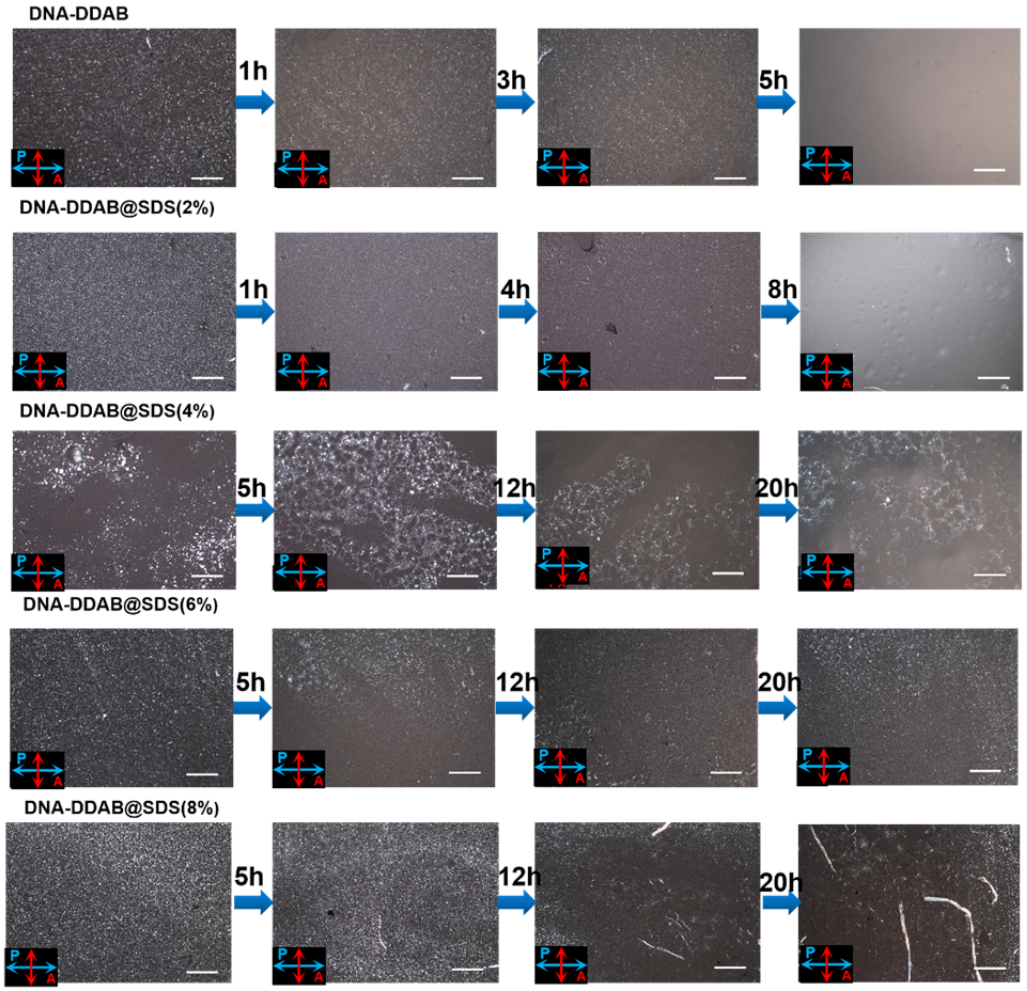

Figure S4. Temporal evolved phase changes of a) DNA-DDAB, b) DNA-DDAB@SDS (2%), c) DNA-DDAB@SDS (4%), d) DNA-DDAB@SDS (6%) and e) DNA-DDAB@SDS (8%) under RH =80% at r.t., recorded by POM analyses. Scale bar: 20 µm.

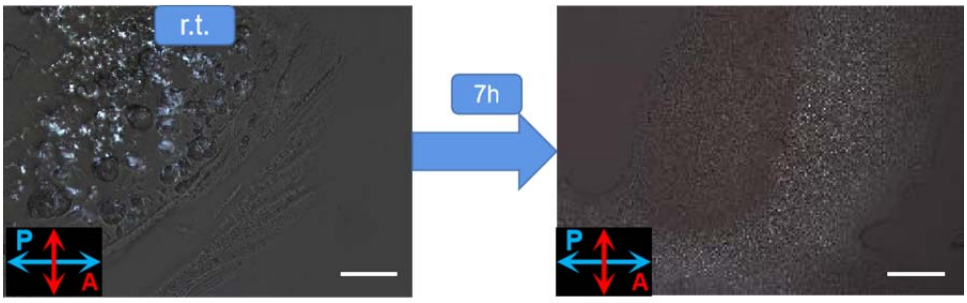

Figure S5. POM analyses on the humidity-induced phase change of DNA-CTAB under RH = 80% at r.t. in 7 h. Scale bar: 20 µm.

Table S1. Mass changes of DNA-DDAB under RH = 80% at r.t.

Time (h)	0	0.5	1	3	5	7	10	20
Weight (mg)	3.0	3.2	3.4	3.8	4.2	4.1	4.1	4.1

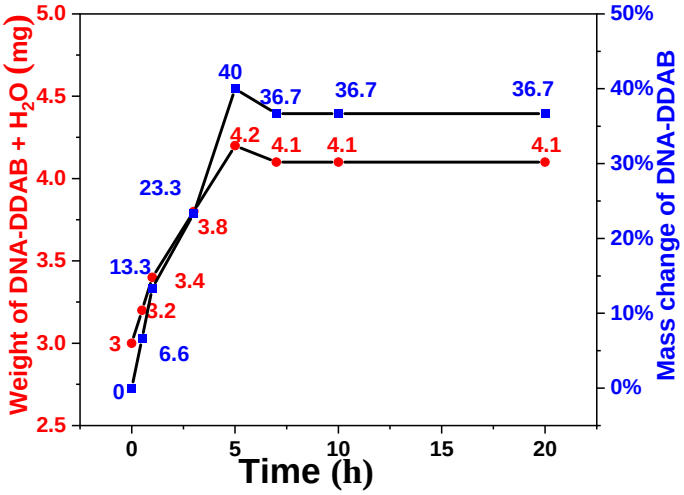

Figure S6. The plotted charts of the mass changes of DNA-DDAB LC under RH = 80% at r.t.

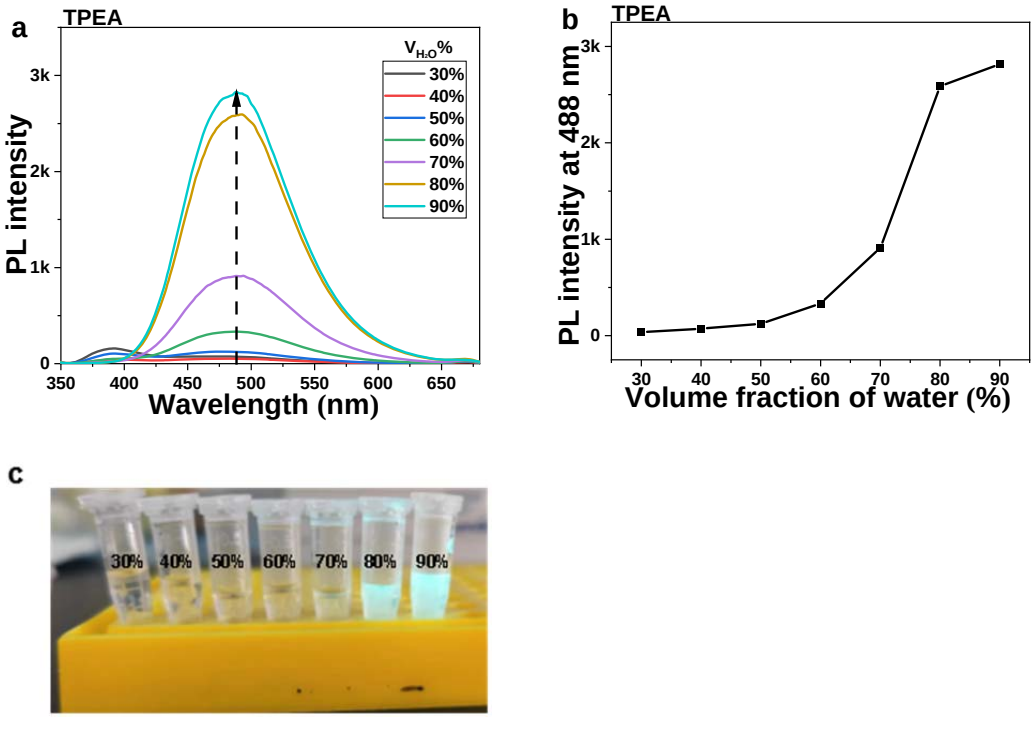

Figure S7. a) PL spectra of TPEA (0.4 mM) in ethanol/H_2O mixture with different volume fractions of H_2O ranging from 30% to 90%. λ_{ex} = 330 nm. b) The plots of PL intensity of TPEA at 488 nm versus the volume fraction of H_2O. c) Fluorescence pictures of solutions or suspensions of TPEA (0.4 mM) in ethanol/H_2O mixture with different volume fractions of H_2O ranging from 30% to 90%.

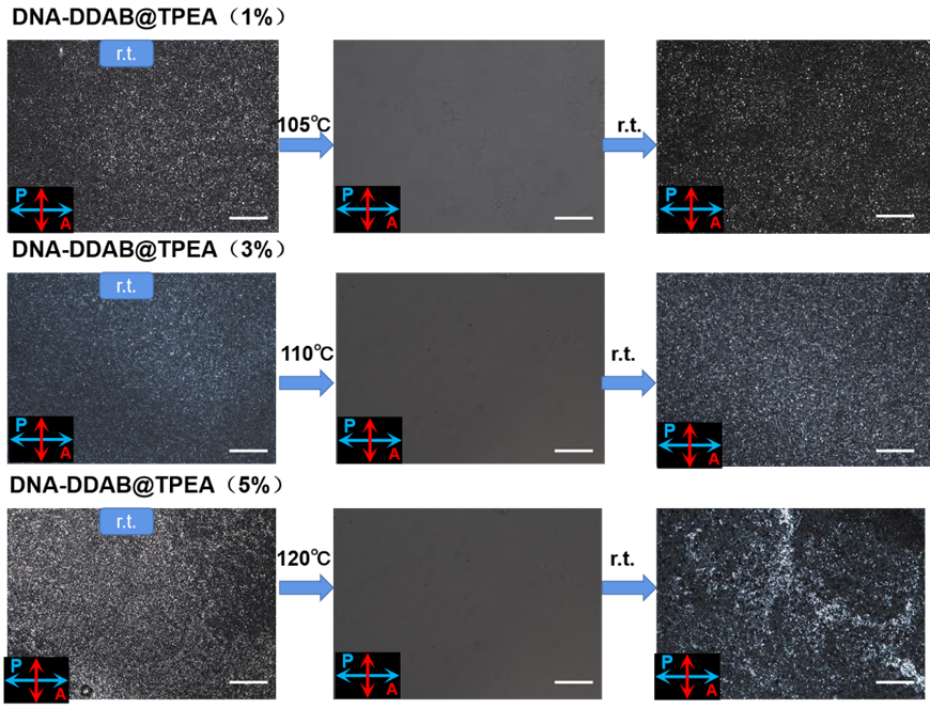

Figure S8. Temperature-dependent POM analyses on the phase changes of DNA-DDAB@TPEA LCs. Scale bar: 20 μm.

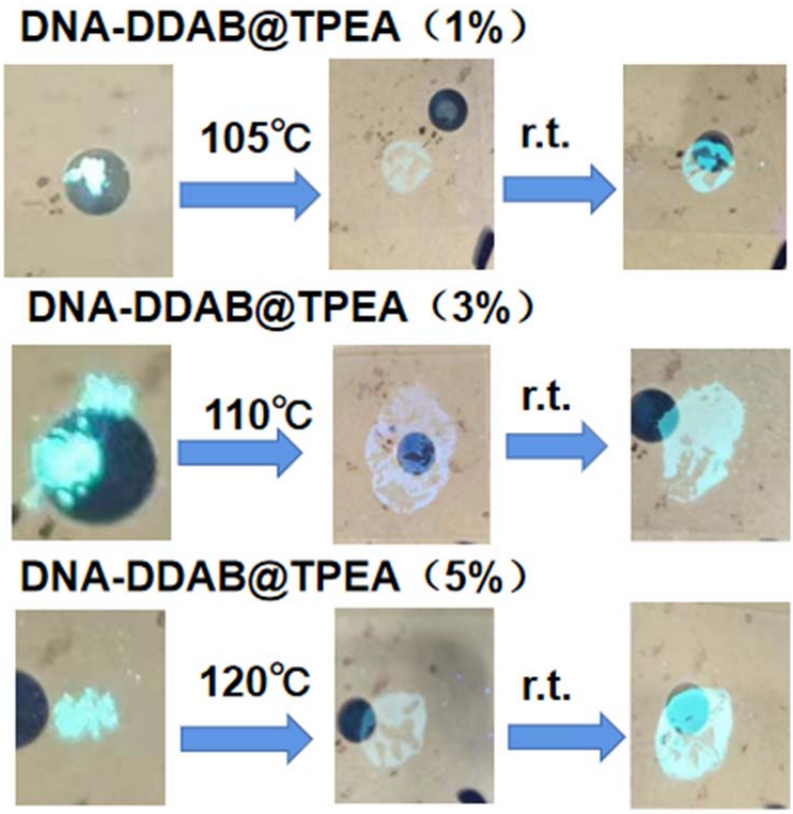

Figure S9. Temperature-dependent fluorescence changes of DNA-DDAB@TPEA LCs.

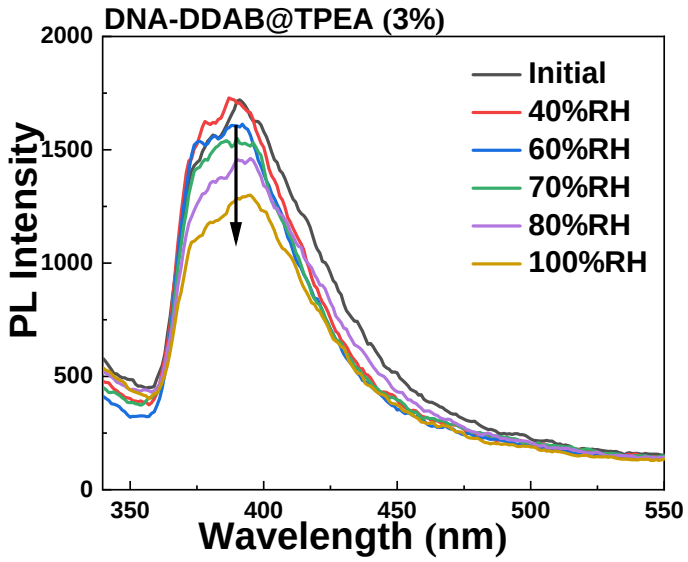

Figure S10. PL spectra of DNA-DDAB@TPEA (3%) under different RHs with 4 min incubation time at r.t. λ_{ex} = 300 nm.

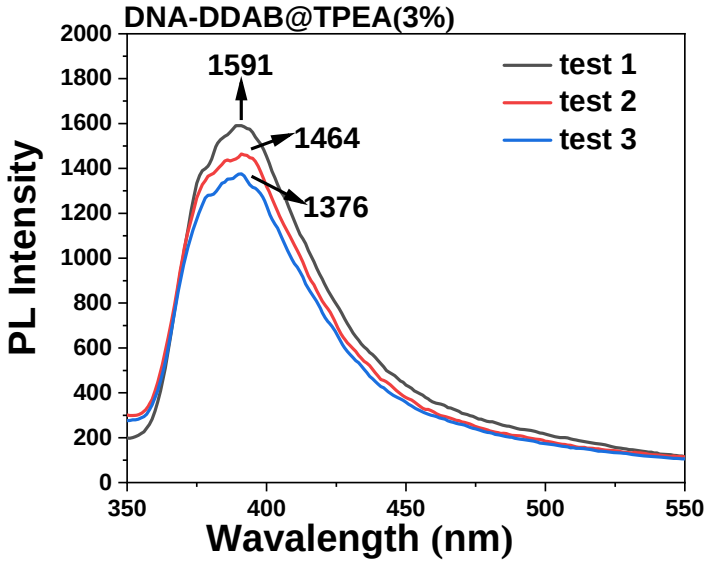

Figure S11. PL spectra of DNA-DDAB@TPEA (3%) under tested environmental conditions with 4 min incubation time. λ_{ex} = 300 nm.

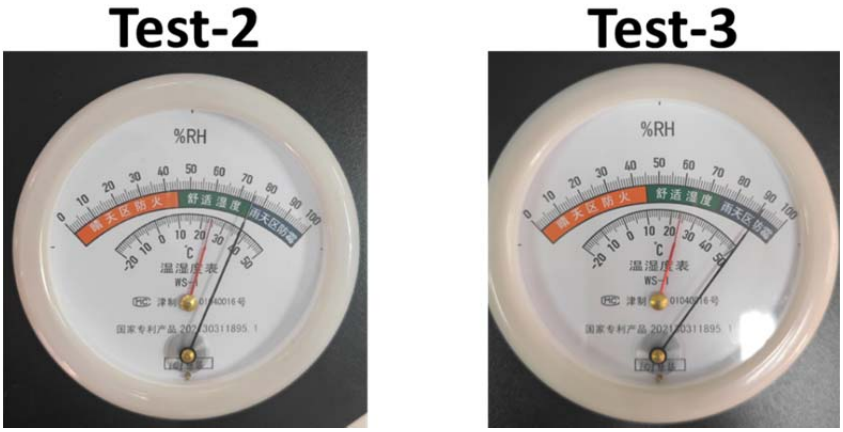

Figure S12. Images of commercial hygrometer at the tested RH conditions at 77% and 90%.

References

1. L. Zhang, C. Zhang, K. Wang, J. Liu, C. Xie and Z. Wu, *Mater. Chem. Front.*, 2022, **6**, 2122-2127.