Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supporting Information

for

Photoresponsive Chiral Vesicles as Light Harvesting Matrix with Tunable Chiroptical Properties

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Experimental section

Materials

All chemicals were purchased from Guoyao Chemical Reagent Co. Ltd, Shanghai, which were used without further purification. CSC was synthesized according to the previous report.[S1]

Characterizations

Transmission electron microscope (TEM) was measured on a JEM-100CX II electron microscope. The samples for TEM detection were dropped in the copper grid and air-dried. CD and CPL were collected with an Applied Photophysics ChirascanV100 model. Emission spectra, life time and quantum yield were measured on a FLS920 Steady State and Transient State Fluorescence Spectrometer. Scanning electron microscope (SEM) images were recorded using a Zeiss scanning electron microscope. The samples for SEM detection were dropped in the silicon pellet, sucking most of solvents by a filter paper and air dried, followed by gold spraying. UV-vis spectra were measured by Agilent ultraviolet visible near infrared spectrophotometer Cary5000. FL spectra were collected by a Shimadzu RF-6000.

Self-assembly

CSC was dissolved in THF as a 10 mM stock solution. Diluting the concentrated solution to deionized water with 10 vol% THF, followed by aging for at least for 8h before subjecting to any characterizations. In order to introducing NR, NR was dissolved in THF as a 10 mM concentrated solution. Taking 1 μL to 5 μL THF solutions of NR to disperse into different self-assemblies (1 ml) in the presence of CSC, samples with NR concentrations of 0.01 mM to 0.055 mM were obtained.

Computational details

The native structures of building units comprising of CSC with different configurations and NR were built from the GaussView06 program, which were initially optimized, and the electrostatic potential (ESP) was simultaneously calculated by Hartree-Fork method. The geometry optimized building units were built by Insert-Molecule modulus into lamellar preassemblies comprising of 66 CSC and 6 NR molecules for the liposome system with a ~3.5 Å *d*-spacing. The water solvent simulated was the SPC216 model. The Antechamber program was used to fit the restrained electrostatic potential (RESP) charge, and then the general Amber force field (GAFF) was adopted to parameterize the for subsequent MD simulations. All MD simulations were implemented with the GROMACS 2020 program. Energy minimization was conducted using the steepest descent algorithm before performing dynamic simulations. MD simulations for system were carried out with a time step of 0.002 ps per integration step under the ensemble conditions of T = 298 K.

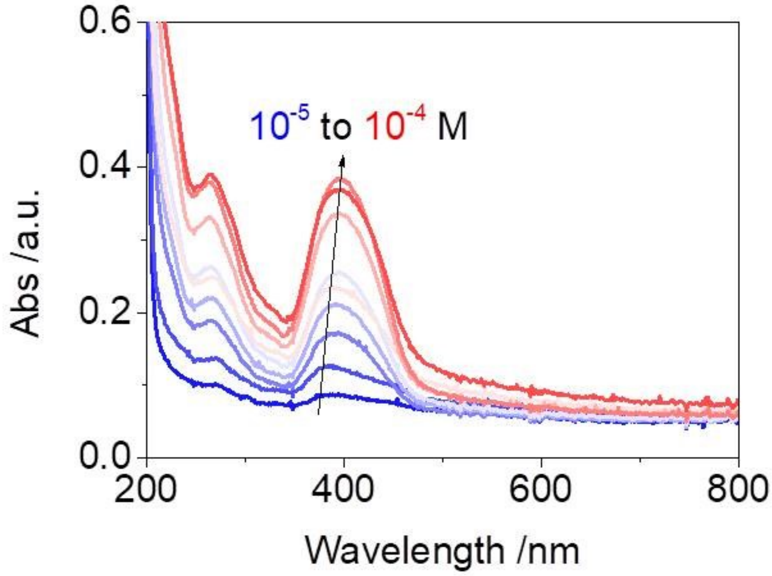

Figure S1. Concentration UV-vis spectra of CSC corresponding to the CD spectra.

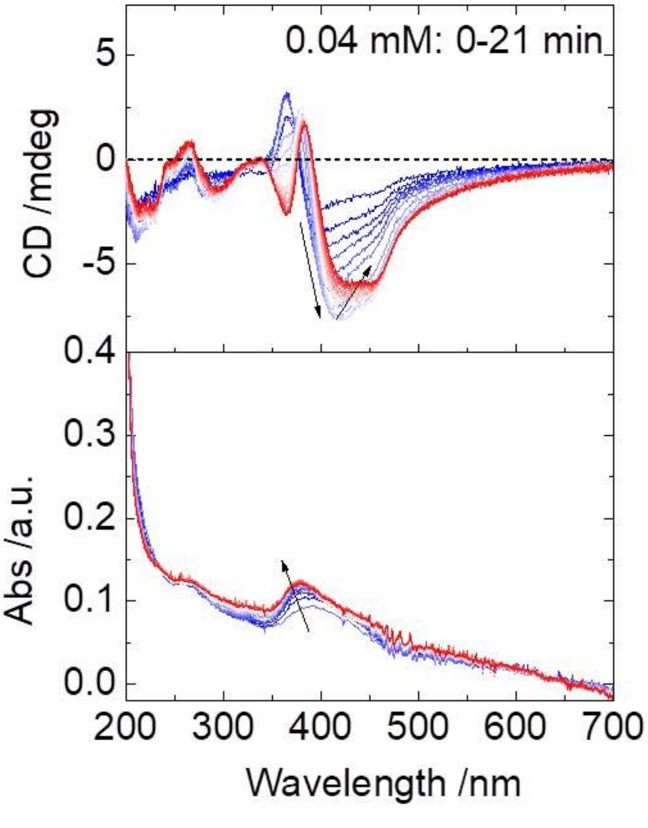

Figure S2. UV light irradiation CD spectra of CSC with a concentration of 0.04 mM. Water fraction = 90 vol%.

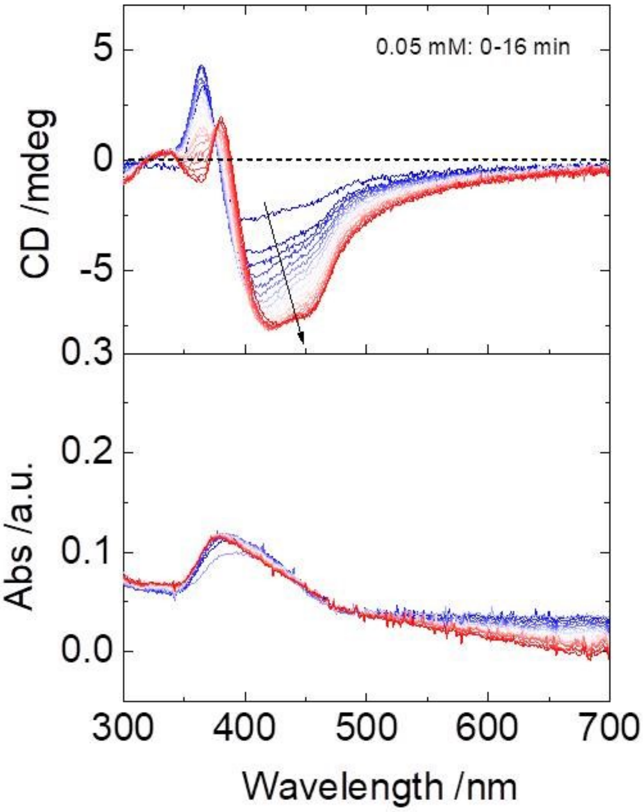

Figure S3. UV light irradiation CD spectra of CSC with a concentration of 0.05 mM. Water fraction = 90 vol%.

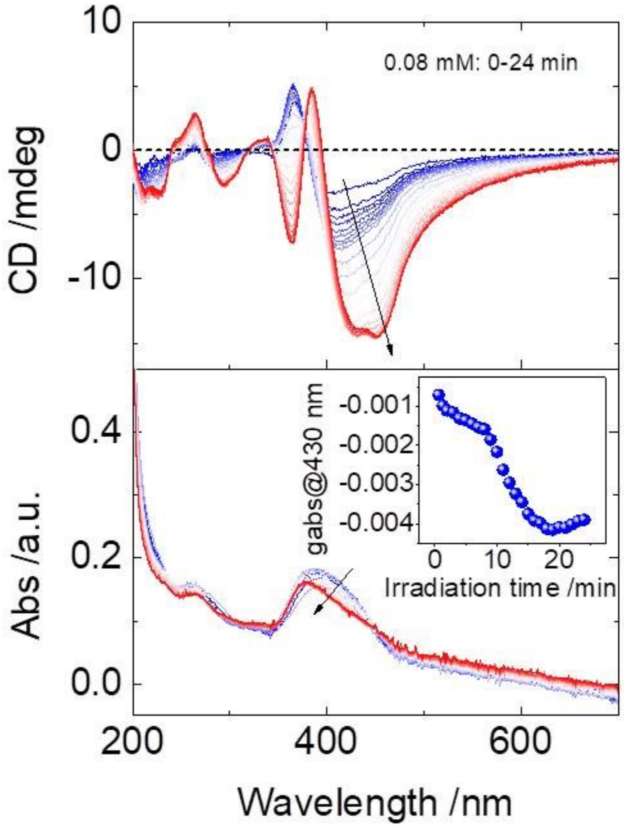

Figure S4. UV light irradiation CD spectra of CSC with a concentration of 0.08 mM. Water fraction = 90 vol%.

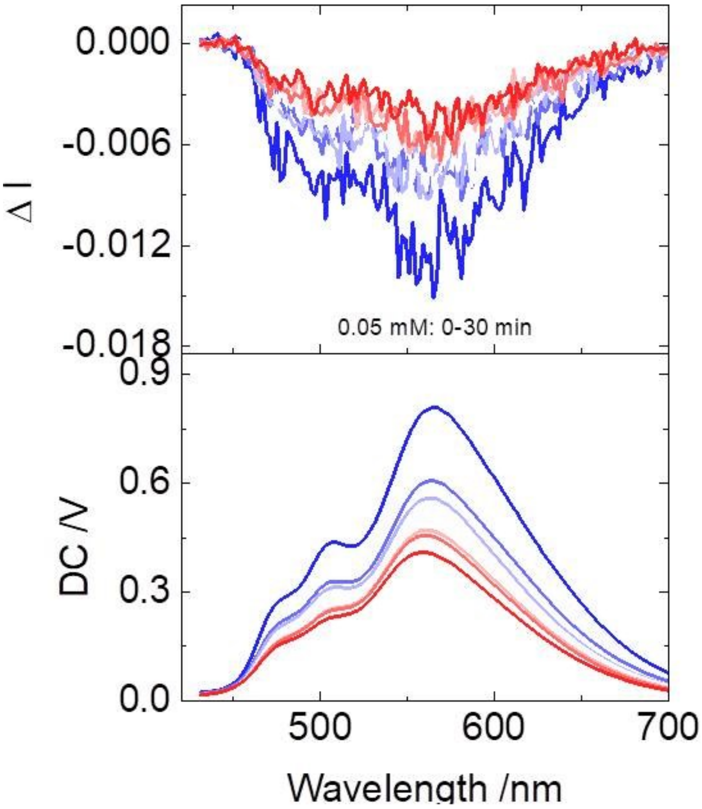

Figure S5. UV light irradiation CPL spectra of CSC with a concentration of 0.05 mM. Water fraction = 90 vol%. Excited at 380 nm.

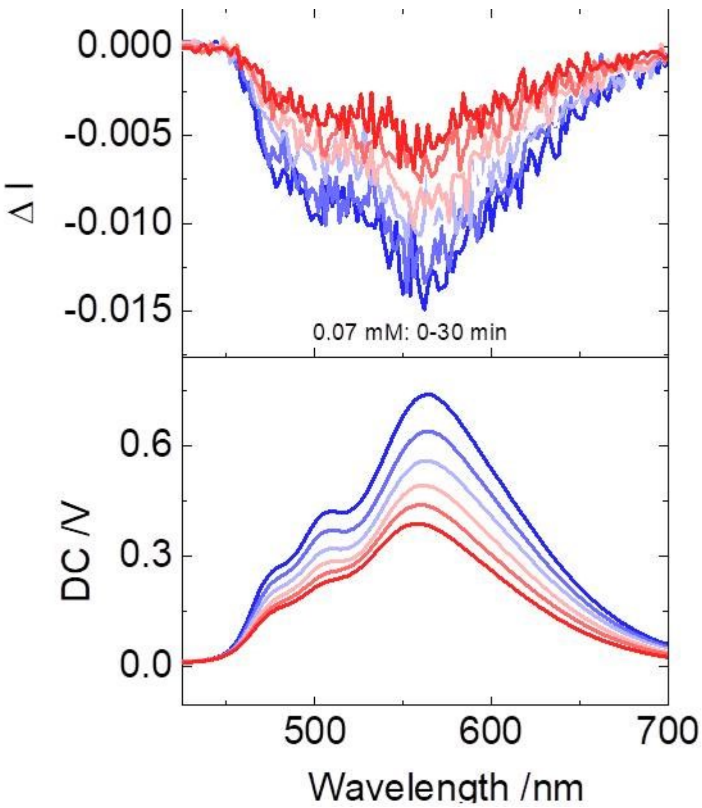

Figure S6. UV light irradiation CPL spectra of CSC with a concentration of 0.07 mM. Water fraction = 90 vol%. Excited at 380 nm.

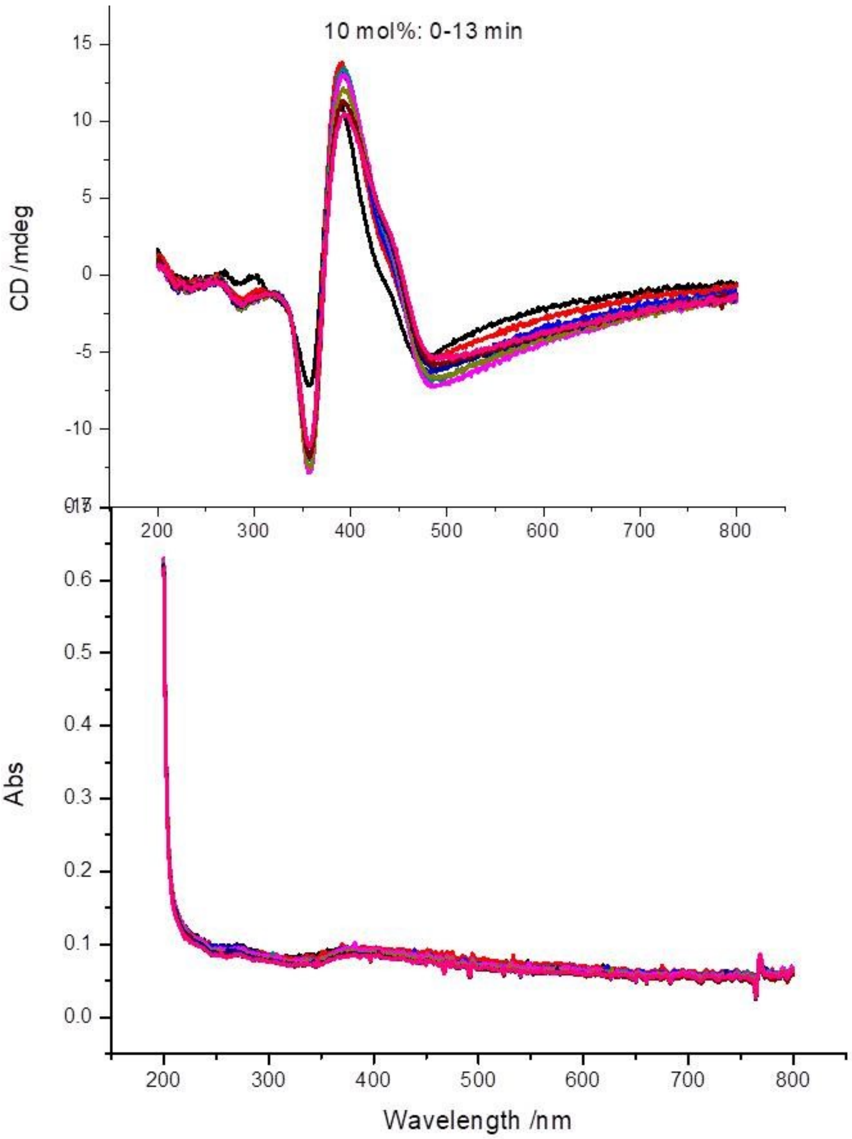

Figure S7. UV light irradiation CD spectra of CSC with a concentration of 0.1 mM with 10 mol% of NR. Water fraction = 90 vol%.

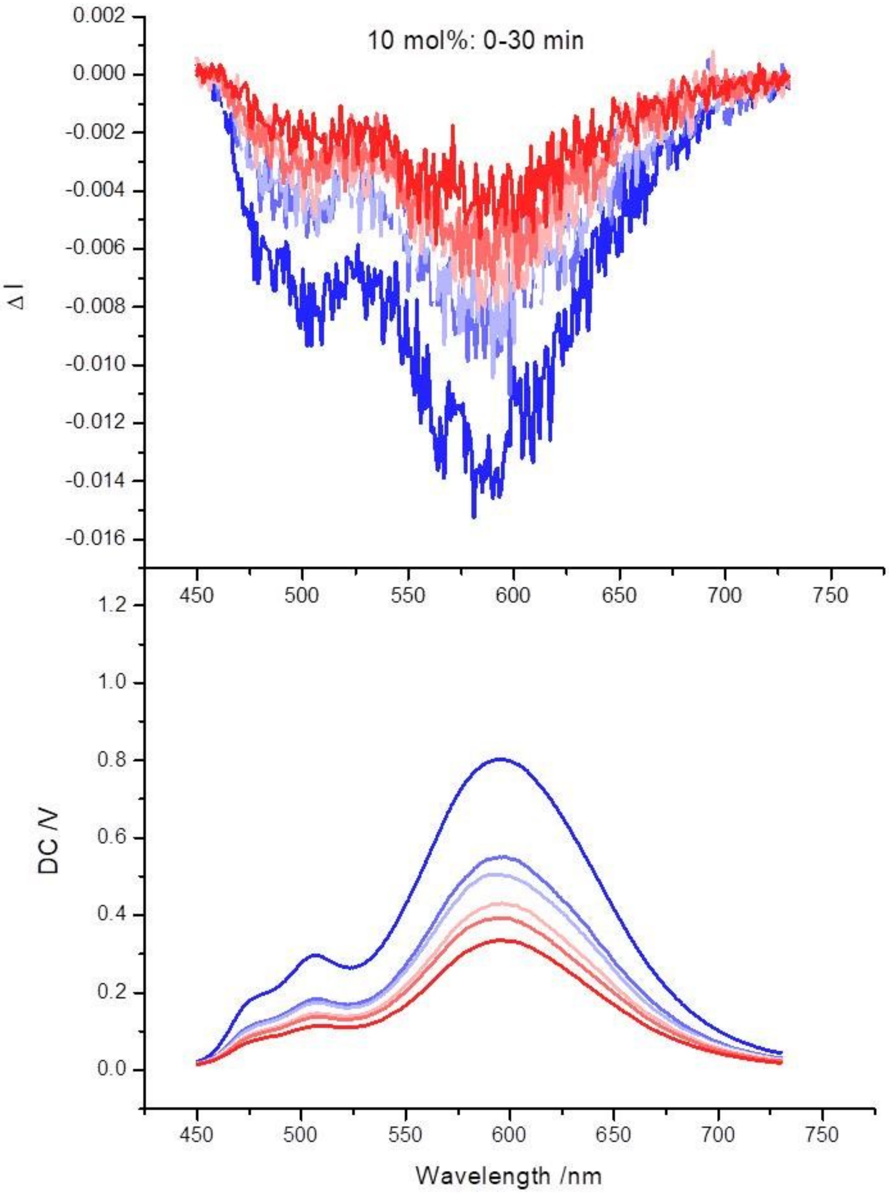

Figure S8. UV light irradiation CPL spectra of CSC with a concentration of 0.1 mM and 10 mol% of NR. Water fraction = 90 vol%. Excited at 380 nm.

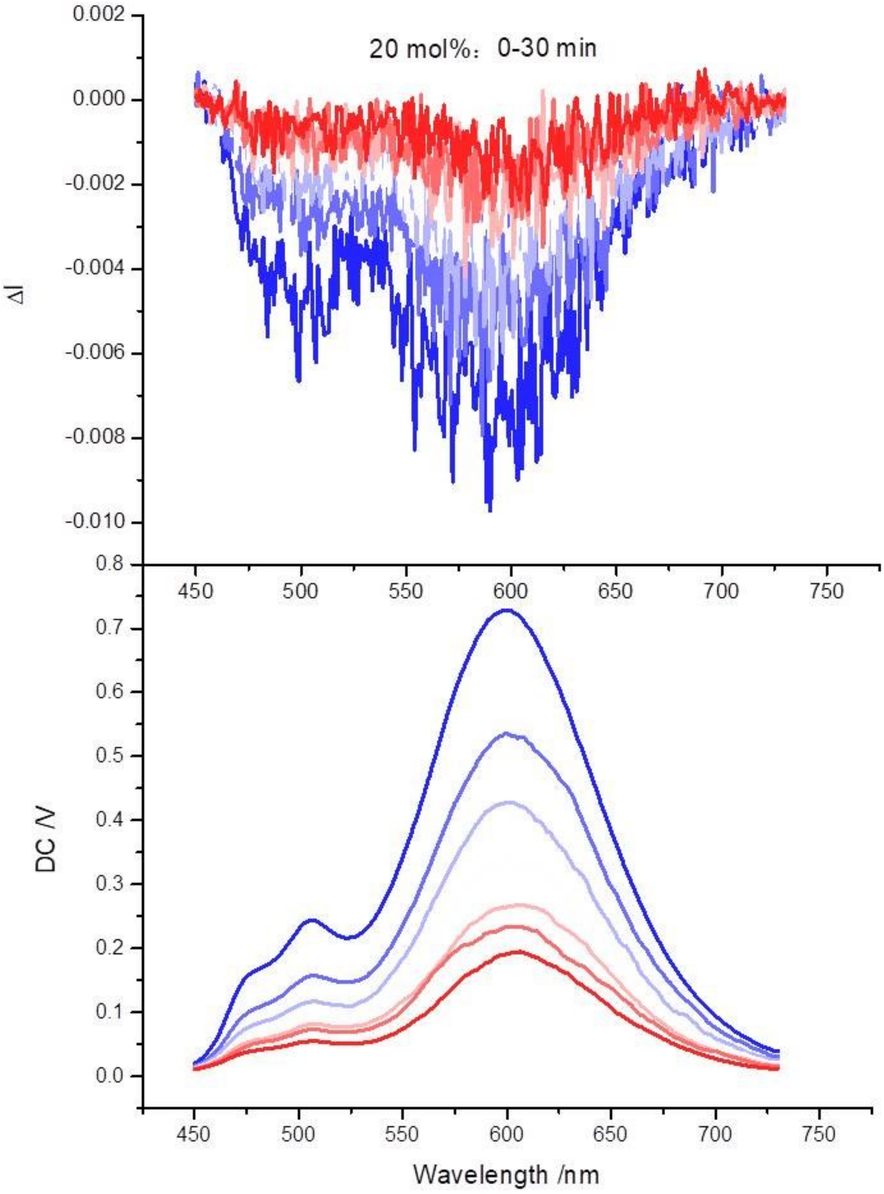

Figure S9. UV light irradiation CPL spectra of CSC with a concentration of 0.1 mM and 20 mol% of NR. Water fraction = 90 vol%. Excited at 380 nm.

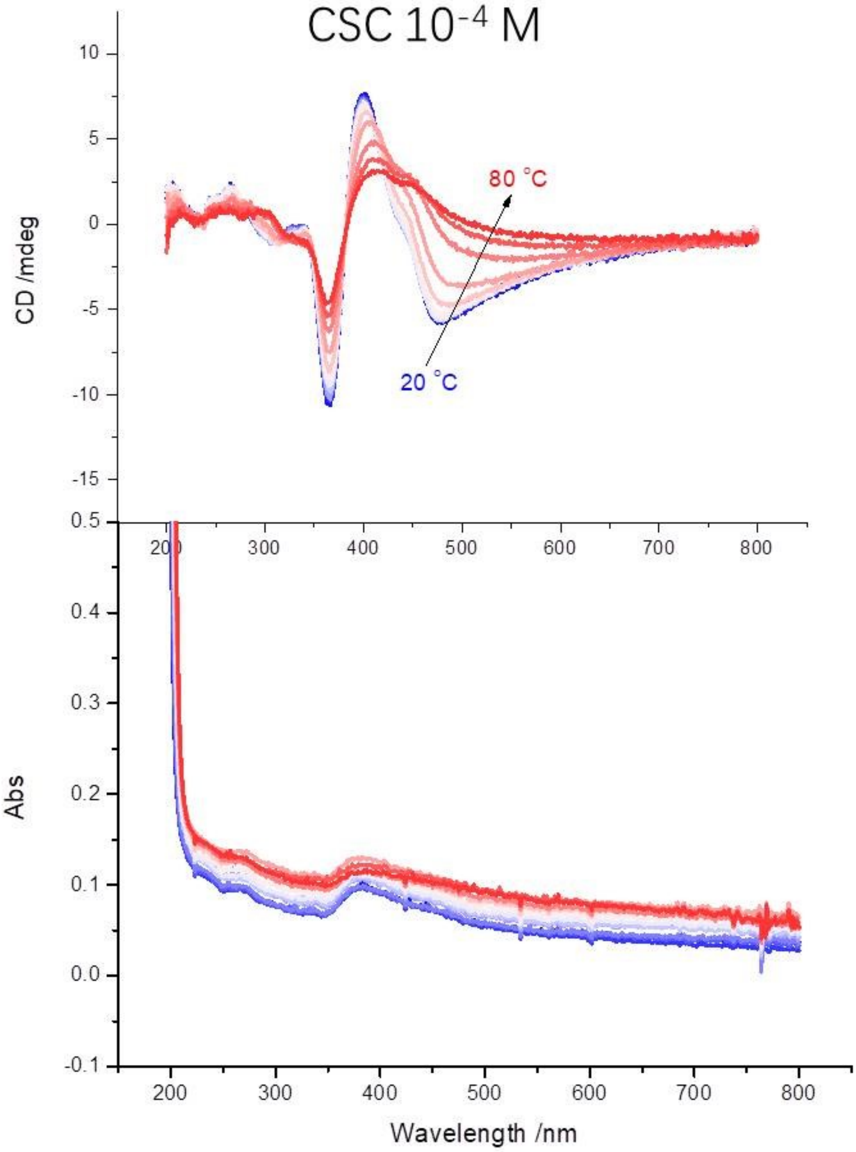

Figure S10. Temperature variable CD spectra of CSC assembly. [CSC] = 10^{-4} M. Water fraction = 90 vol%.

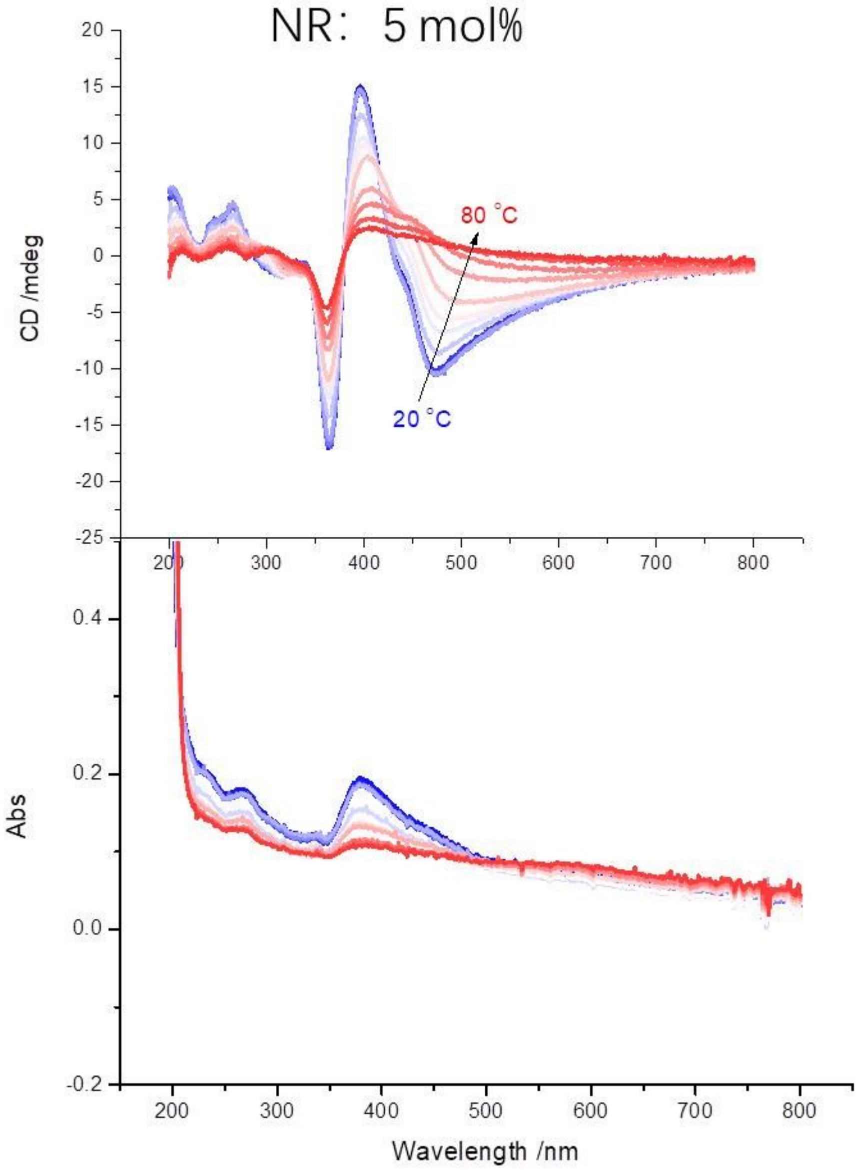

Figure S11. Temperature variable CD spectra of CSC assembly with 5 mol% of NR. [CSC] = 10^{-4} M. Water fraction = 90 vol%.

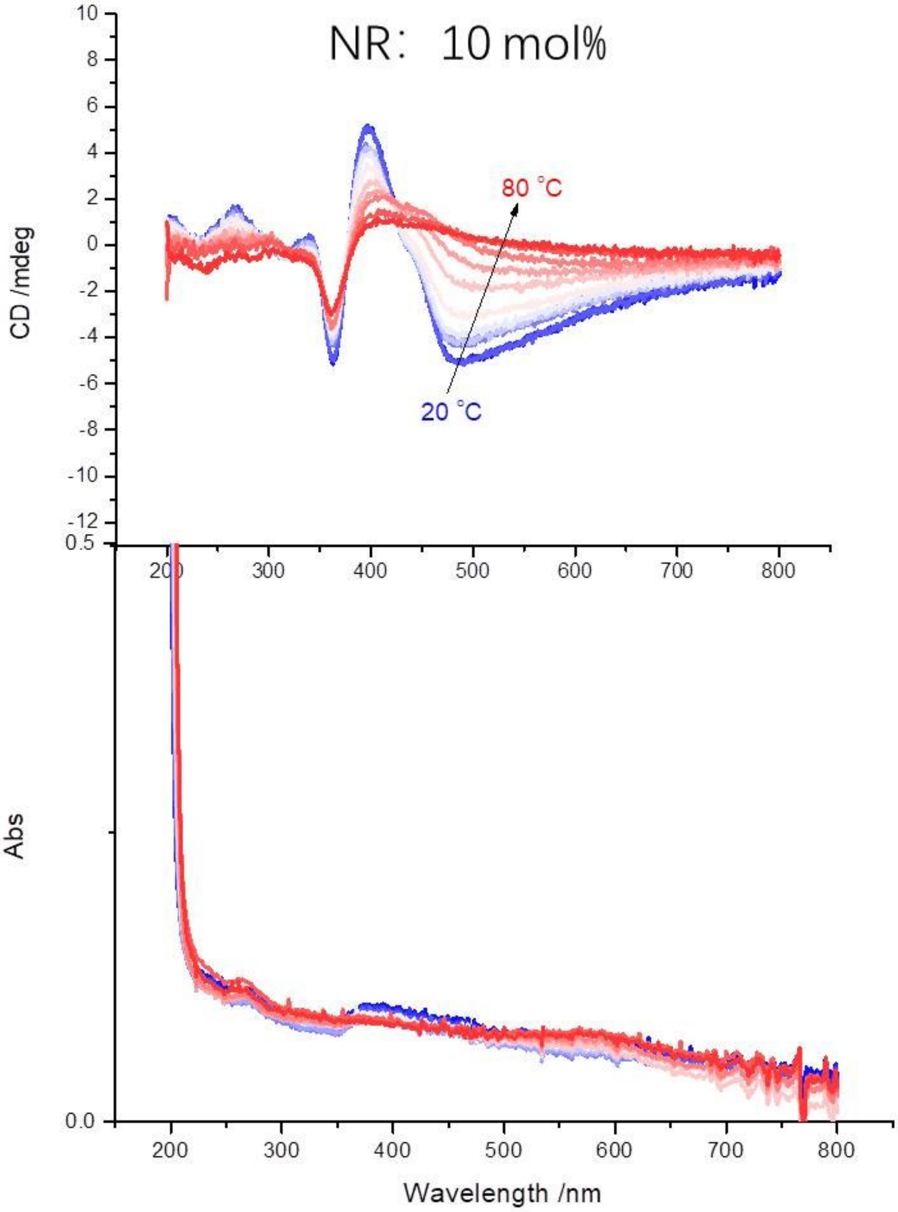

Figure S12. Temperature variable CD spectra of CSC assembly with 10 mol% of NR. [CSC] = 10^{-4} M. Water fraction = 90 vol%.

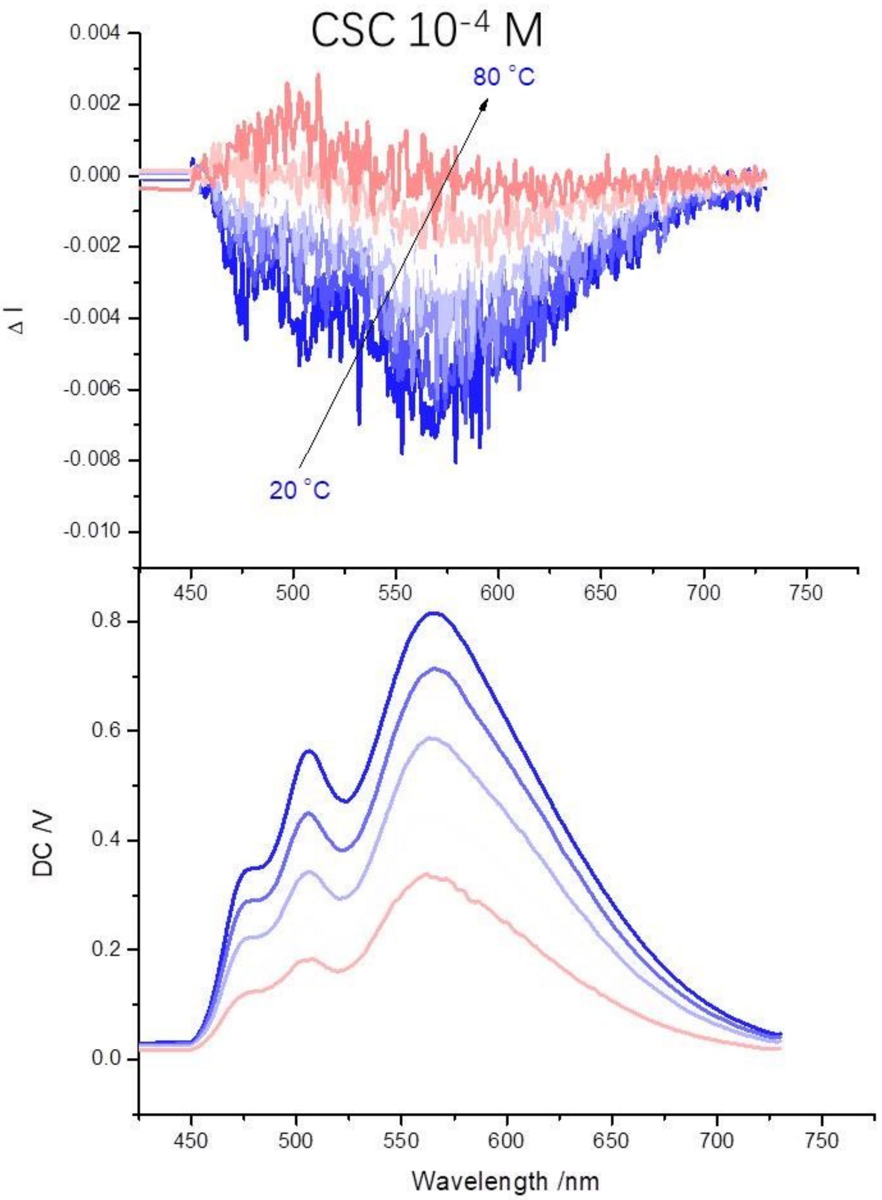

Figure S13. Temperature variable CPL spectra of CSC assembly. [CSC] = 10^{-4} M. Water fraction = 90 vol%. Excited at 380 nm.

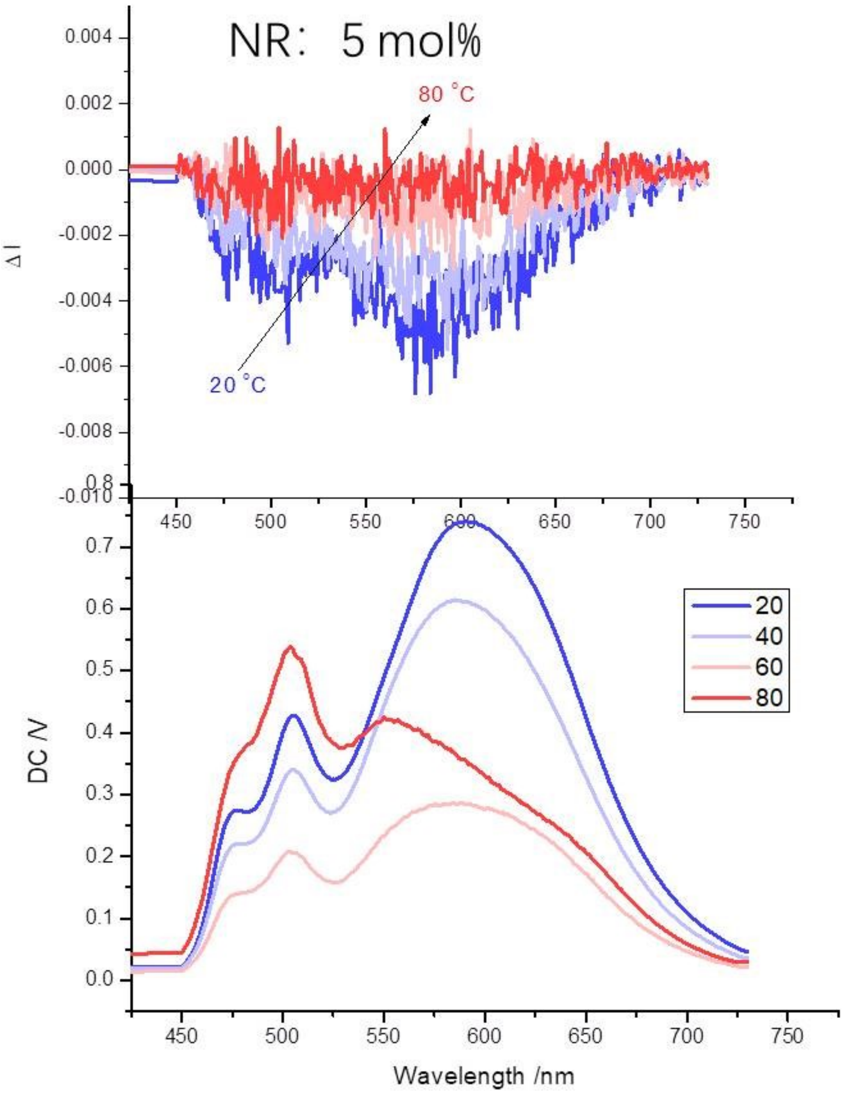

Figure S14. Temperature variable CPL spectra of CSC assembly with 5 mol% of NR. [CSC] = 10^{-4} M. Water fraction = 90 vol%. Excited at 380 nm.

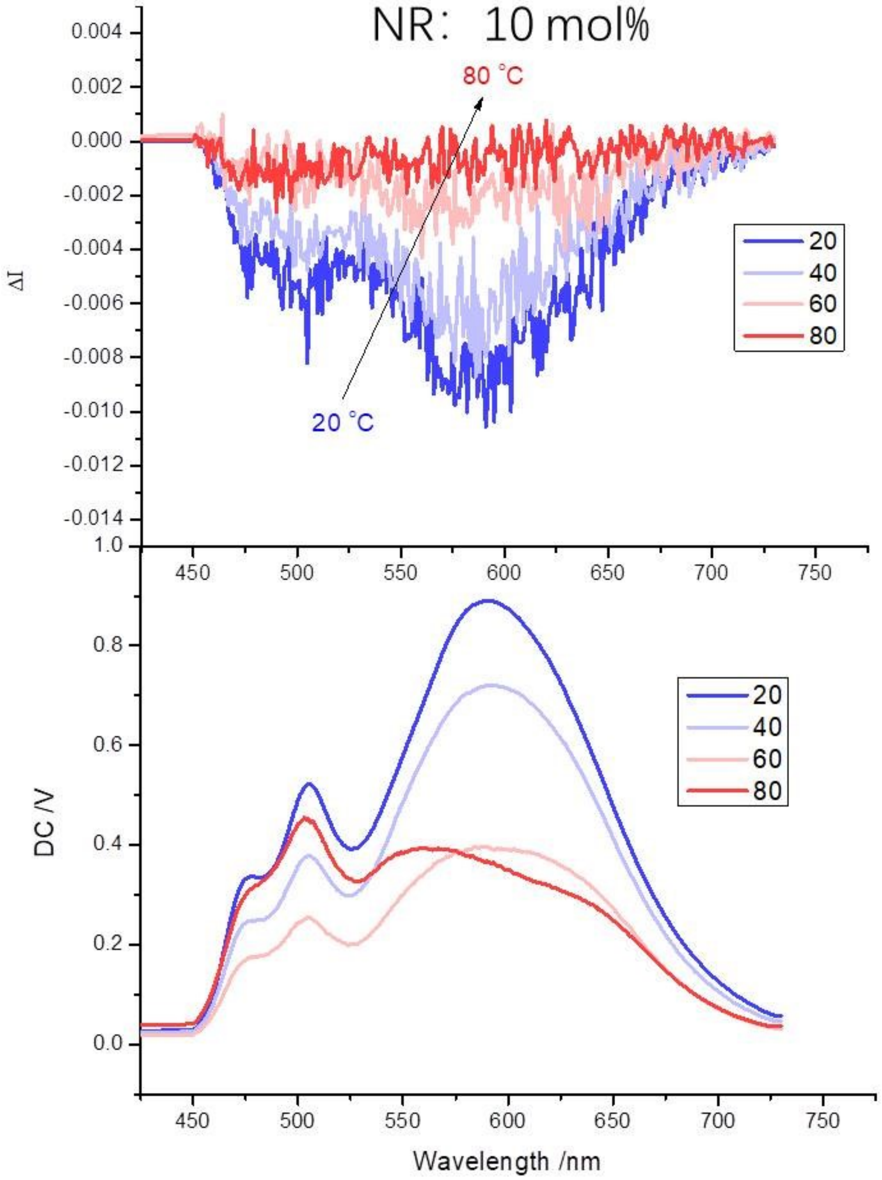

Figure S15. Temperature variable CPL spectra of CSC assembly with 10 mol% of NR. [CSC] = 10^{-4} M. Water fraction = 90 vol%. Excited at 380 nm.

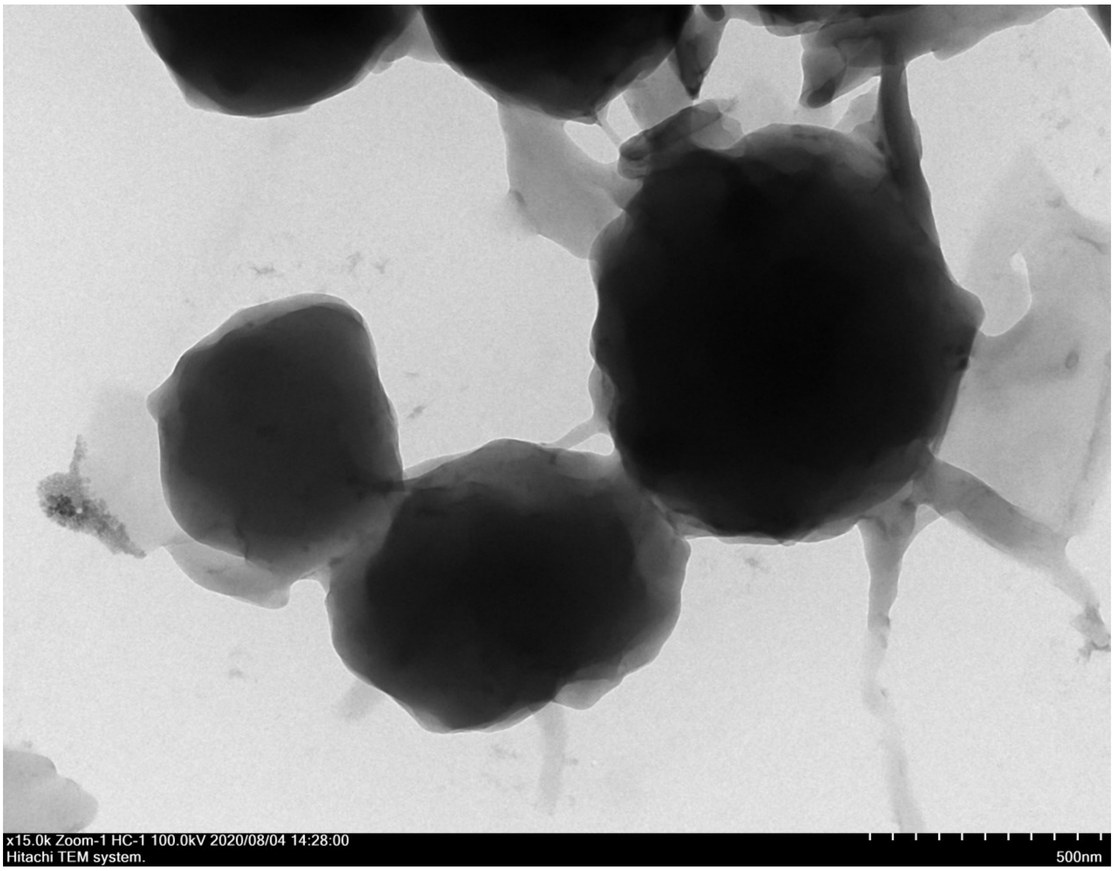

Fig. S16 TEM image of CSC assembly with 5 mol% NR.

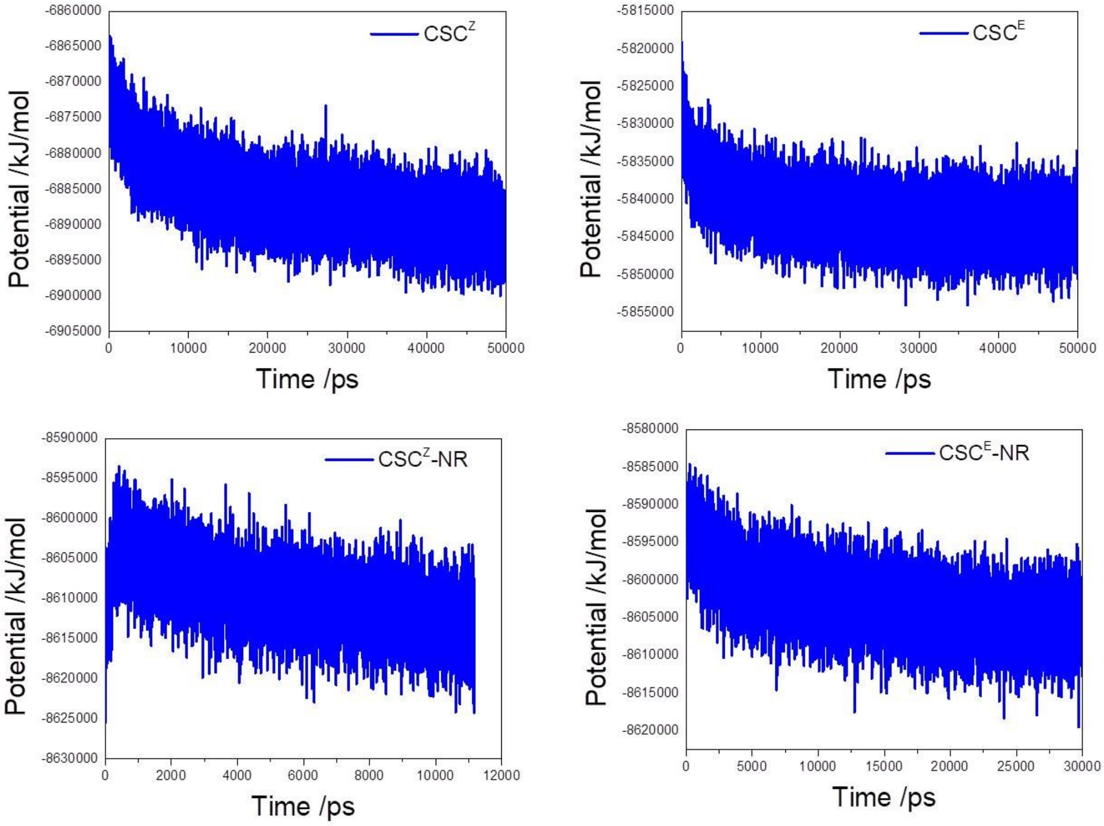

Figure S16. Potential changes of different systems with simulation time.

References

S1. P. Xing, H. Chen, L. Bai and Y. Zhao, *Chem. Commun.*, 2015, **51**, 9309.