Electronic Supplementary Material (ESI) for RSC Advances.

Spontaneous formation and the reversible transformation of achiral J-aggregates and chiral H-aggregates

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1. Material and reagents

The cyanine dye (MTC) was synthesized according to Hamer[1] and Fichen's[2] methods, and the purity was proved by Mass Spectra, Nuclear Magnetic Resonance and Elemental Analysis techniques. And all other reagents were purchased from commercial sources and used without further purification.

2. Spectral measurement

Absorption and CD spectra were taken on a UV-1601PC spectrophotometer and a JASCO J-815 spectrophotometer, respectively, in a 10-mm quartz cells at room temperature. All CD spectra were collected at 500 nm/min, with five scans averaged.

(a) (b)

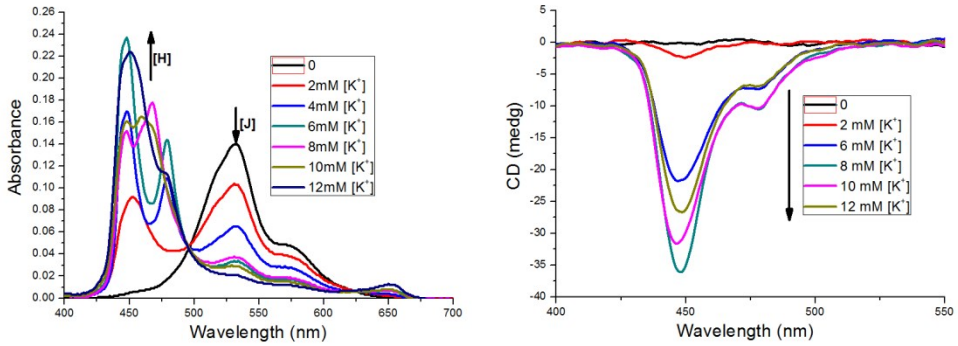

Fig. S1. Uv-vis spectra (a) and CD spectra (b)of MTC self-aggregates in 5 μM dependent on the titration of KCl.

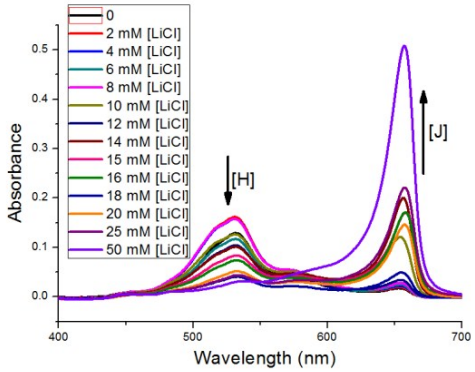

Fig. S2. Uv-vis spectra of MTC self-aggregates in 5 μM dependent on the titration of LiCl.

3. DLS measurement

Dynamic light scattering (DLS) measurements were carried out by non-invasive backscattering on an ALV/CGS-3 compact goniometer system with an ALV/LSE-5003 and a multiple tau correlator at a wavelength of 632.8 nm (He–Ne Laser) and a goniometer angle of 90°. The dispersing media were purified before use with a syringe-filter (200 nm mesh). The determination of the particle size was carried out by the analysis of the correlation-function via the g2(t) method followed by a linearised number-weighting (n.w.) and mass weighting (m.w.) of the distribution function.

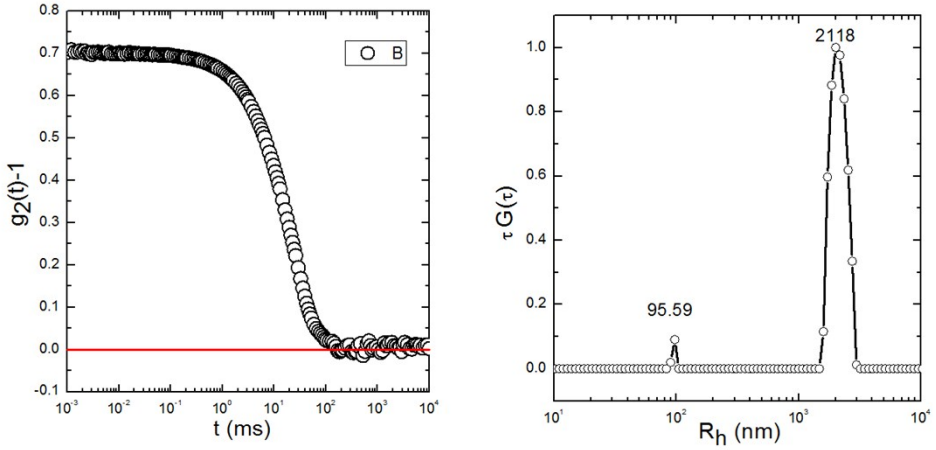

Fig. S3. DLS datas of achiral J-aggregates.

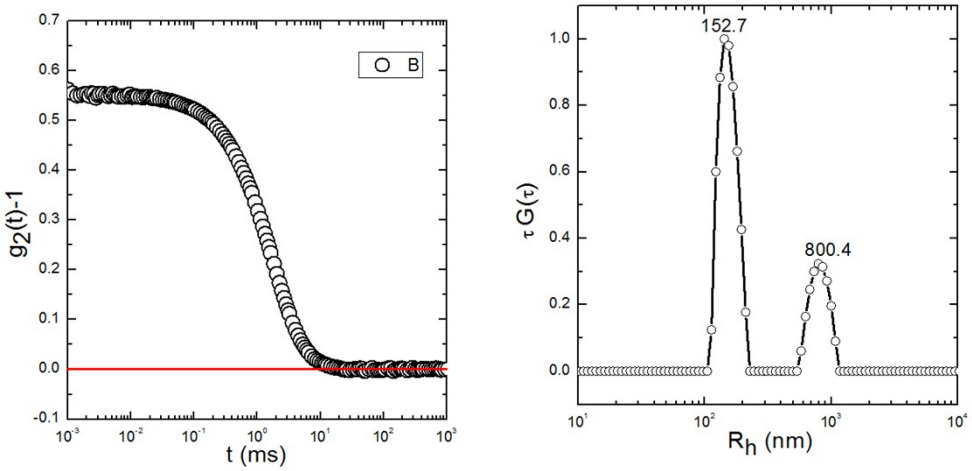

Fig. S4. DLS datas of chiral H-aggregates.

4. TEM measurement

TEM images were conducted at 200kV using a JEOL TEM JEM-2011. The samples were attached to Formvar copper grids by dispersing them in ethanol using an ultrasound cleaning bath, adding one drop on the copper grid and evaporating the solvent. The images were evaluated automatically by the software ImageJ or manually in the case of a very low contrast.

5. ^{23}Na-NMR measurement

NMR spectra were obtained with a Bruker Avance II+400 spectrometer equipped with 5mm BBO probe operating at the Fourier transform mode of resonance signals, and the accumulated signals provoked by radio-frequency pulses of 90^{o} were recorded.

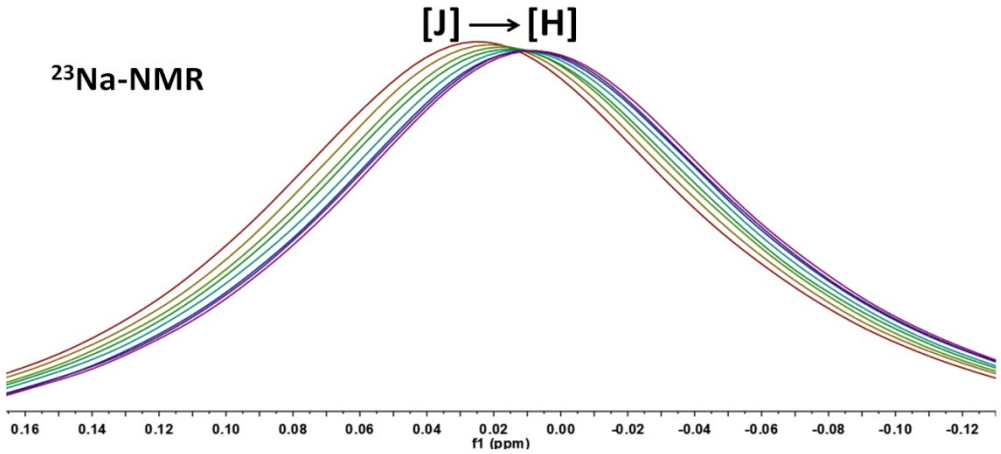

Fig. S5. ^{23}Na-NMR signals during the transformation from the MTC J-aggregates [J] to chiral H-aggregates [H] within 4 hours, the datas were accumulated at intervals of half an hour.

References:

[1] F. M. Hamer, *The chemistry of heterocyclic compounds*, 1964.

[2] G. E. Ficken, *The chemistry of synthetic dyes,* 1971.