Electronic Supplementary Information (ESI)

Structural change from homogenous structure to staging in benzoic acid intercalated LDH: experimental and molecular dynamics simulation insights

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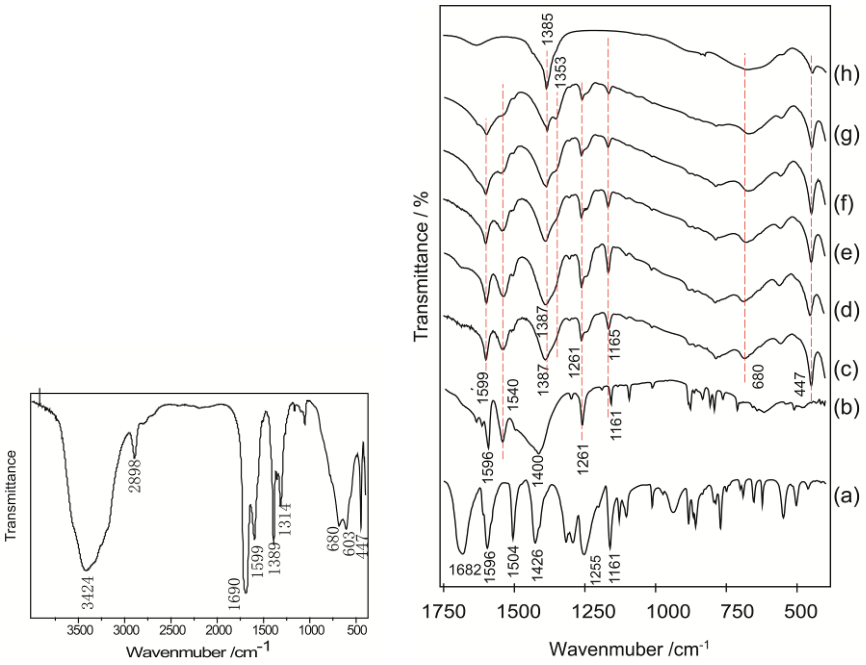

Fig. S1 (A) FT-IR spectrum of C-0.25 in formamide (B) FT-IR spectra of (a) OBA raw material, (b) OBA deprotonated with NaOH, and the water-washed samples (c) C–2, (d) C–1, (e) C–0.5, (f) C–0.25, (g) C–0.125, and (h) NO_3^--LDH after drying at 100 °C *in vacuo*.

In the spectra, the bands at 1682 and 1426 cm^{-1} were assigned to characteristic absorption band of carboxyl group (–COOH) in OBA molecule. They shifted to lower wave numbers at 1596 and 1400 cm^{-1}, corresponding to the ν_{as} and ν_s vibrations of $–COO^-$ in OBA^{2-} anions. The presence of the vibrations of benzene ring at 1540 cm^{-1}, and the Mg(Al)–O stretching vibrations at 680 and 447 cm^{-1} suggested that the coassembly of OBA^{2-} with LDH. The bands of 1384 and 1354 cm^{-1} are characteristic of NO_3^- and CO_3^{2-}, respectively. The former is shown for the NO_3^--LDH (Fig. S1B-h), C–0.5, C–0.125 and C–0.25 samples, but is not distinct for C–2 and C–1 because the band at 1387 cm^{-1} may be due to the ν_s vibration of $–COO^-$. The CO_3^{2-} band at 1354 cm^{-1} could be found in the patterns of C–0.125 and C–0.25, but became a shoulder for other samples.

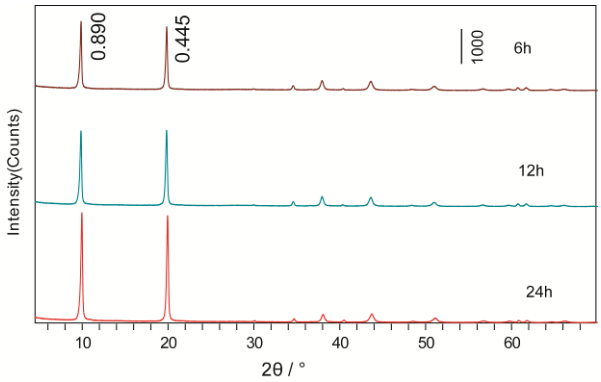

Fig. S2 XRD patterns of the samples NO_3^-–LDH heating at 100°C for 24 h, 12 h and 6 h, respectively; *d*–value in nanometers.

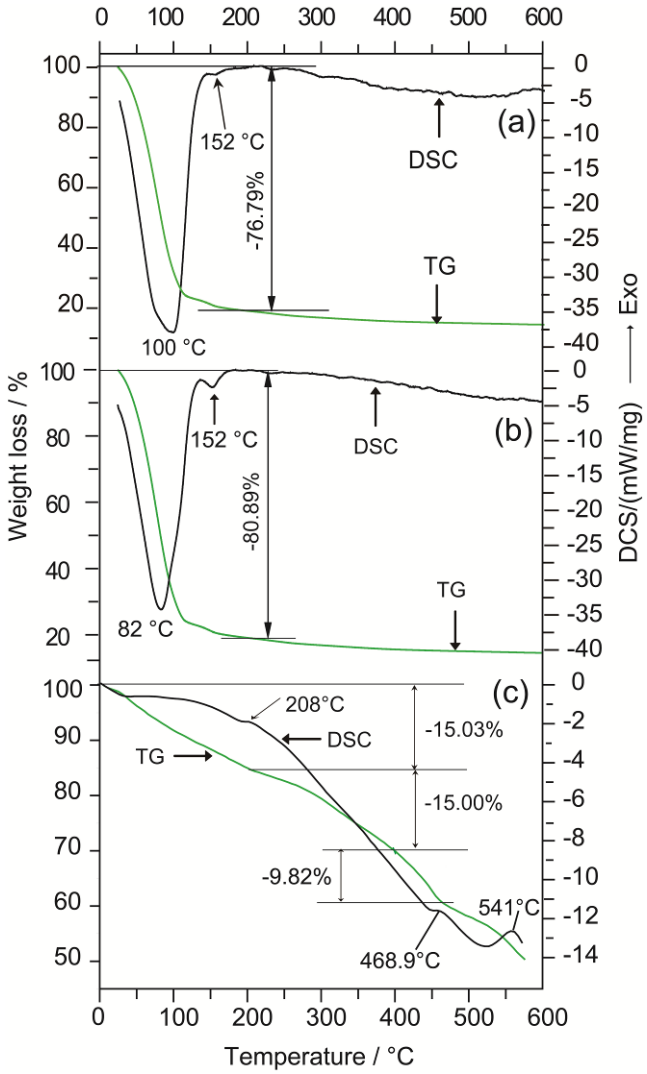

Fig. S3 TG and DSC curves of (a) C–1 and (b) C–0.25 in wet state after water–washing, and (c) C–0.25 drying at 100 °C *in vacuo*.

The TG curves exhibited that water lost in a large amount during heating till 100 °C and became smaller from 100 to ~200 °C corresponding to two endothermic peaks in DSC curves, respectively.

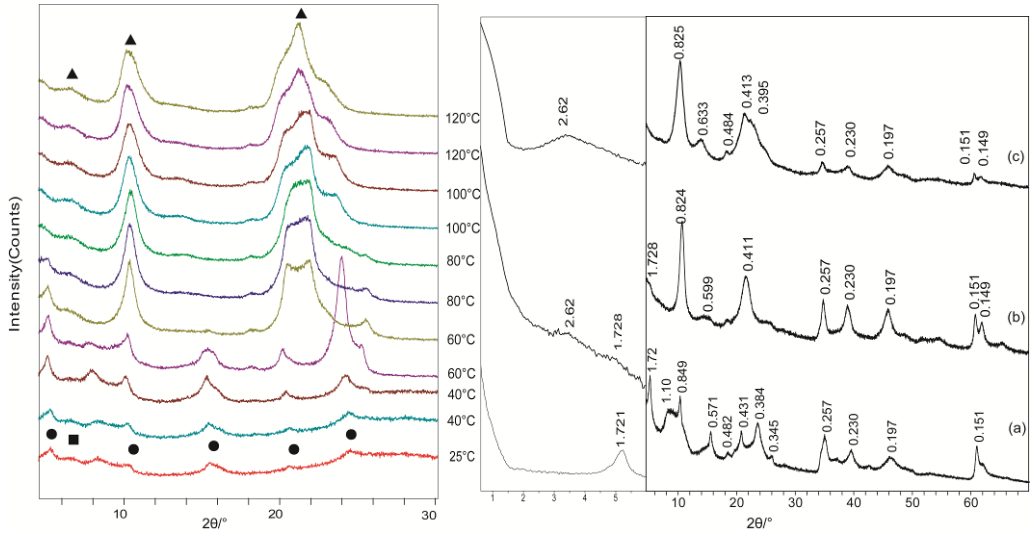

Fig. S4 (A) *In situ* XRD patterns of C-0.25 in the temperature range 25-120°C (B) XRD patterns of the sample at different drying temperatures (a) 40 °C, (b) 80 °C, (c) 120 °C; *d*–value in nanometers.

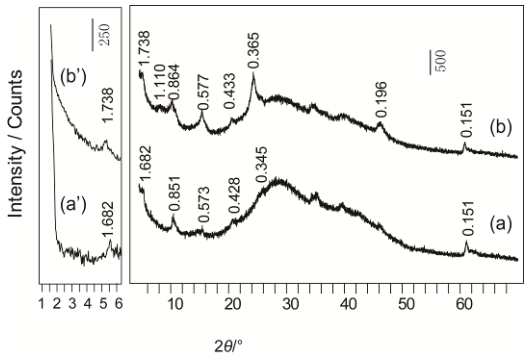

Fig. S5 XRD patterns of (a, a') C-1 and (b, b') C-0.25 after the dried samples immersed in degassed water for 24 h; *d*–value in nanometers.

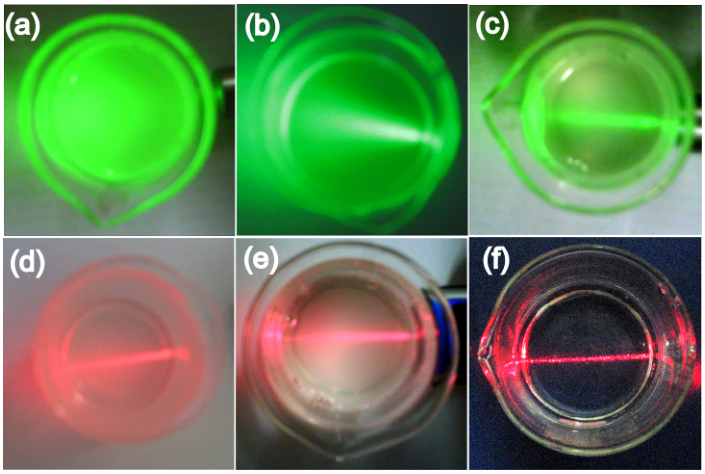

Fig. S6 Tyndall light scattering behaviours of the samples of (a) C–2, (b) C–1, (c) C–0.5, (d) C–0.25 and (e) C–0.125 after OBA^{2-} added into the colloidal suspension of LDH in formamide (f).

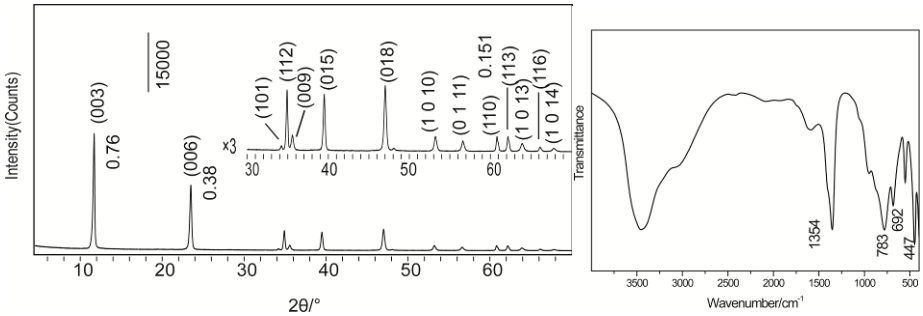

Fig. S7 XRD pattern and FT-IR spectrum of CO_3^{2-}–LDH; *d*–value in nanometers.

In the XRD pattern of the CO_3^{2-}–LDH sample, all the diffraction peaks could be indexed to a hexagonal symmetry with the lattice parameters a = 0.30444(1), c = 2.27059(8) nm. In the FT-IR, the bands at 1354 was the characteristic of CO_3^{2-}.

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