Electronic Supplementary Information

Formation of silicate nanoscrolls through solvothermal treatment of layered octosilicate intercalated with organoammonium ions

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Contents

Crystallographic data of Layered Octosilicate

The following data were obtained from the literature.[1]

Unit cell	
Space group	$I4_1/amd$
a	7.3276 Å
c	44.319 Å
cell content	$Na[Si_4O_8(OH)]\cdot 4H_2O$

Fractional Coordinates

atom	Wyckoff letter	*x*	*y*	*z*	B_{eq}
Si1	16g	0.289(1)	0.039(1)	1/8	1.5
Si2	16h	0	0.544(1)	0.074(1)	1.5
O1	32i	0.171(1)	0.987(1)	0.096(1)	3.1
O2	16h	0.253(1)	1/4	0.134(1)	3.1
O3	8e	0	3/4	0.062(1)	3.1
O4	16h	0	0.093(1)	0.045(1)	3.5
Na	8e	1/2	1/4	0.002(1)	6.0
O5 (H_2O)	16f	0.254(1)	1/2	0	4.0
O6 (H_2O)	8e	1/2	3/4	0.053(1)	4.0
O7 (H_2O)	8e	1/2	1/4	0.051(1)	4.0

1. S. Vortmann *et al.*, *J. Phys. Chem. B*, **101**, 1292 (1997)

Equation for the calculation of sheet size forming one nanoscroll

$$D_n = D + d \times (n - 1) \times 2 \qquad (1)$$

$$L = \sum_{n=1}^{13} \pi D_n \qquad (2)$$

D [nm]: inner diameter of a nanoscroll

n: the number of the layer stacking

(the number of layer stacking of one typical nanoscroll is 13)

D_n [nm]: diameter of n-th layer of hypothesized multiwall nanotube

d [nm]: distance between the stacking layers in a wall

L [nm]: sheet size forming one nanoscroll

Table S1. Elemental analysis data.

	C / wt%[a]	H / wt%[a]	N / wt%[a]	SiO_2 / wt%[b]	Na /wt%[c]	C/N	N/Si	Na/Si	Br/Si[d]
Na-Oct	-	-	-	29.5	5.1	-	-	0.21	-
$(C_{18})_2$DMA-Oct	54.1	10.5	1.7	31.3	0.067	37.8	0.23	0.007	0.07
solvo_$(C_{18})_2$DMA-Oct	49.2	9.3	1.6	38.9	-	36.8	0.17	-	0.03

[a]The values were collected by CHN analysis.

[b]A residual amount after thermogravimetry up to 900 °C is regarded as the amount of silica in the samples.

[c]The values were collected by ICP analysis.

[d]The values were determined by EDX analysis.

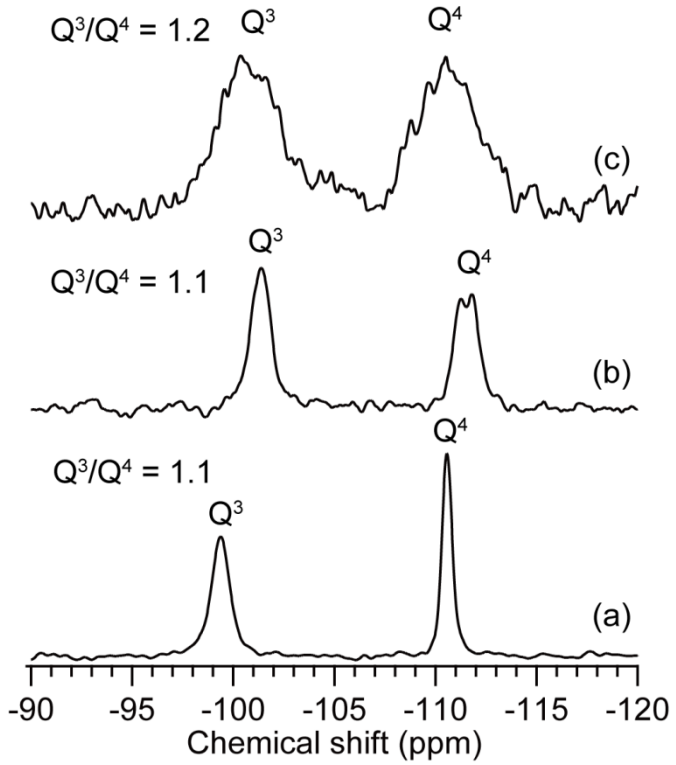

Fig. S1 ^{29}Si MAS NMR spectra of (a) Na-Oct, (b) $(C_{18})_2$DMA-Oct, and (c) solvo-$(C_{18})_2$DMA-Oct.

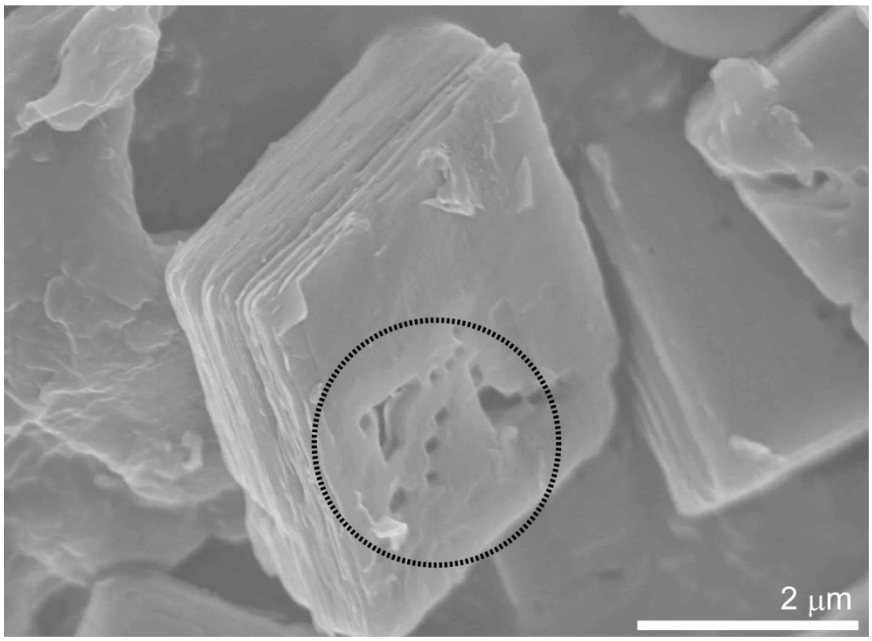

Fig. S2 SEM image of another view of $(C_{18})_2$DMA-Oct. The circle shows defective sites.

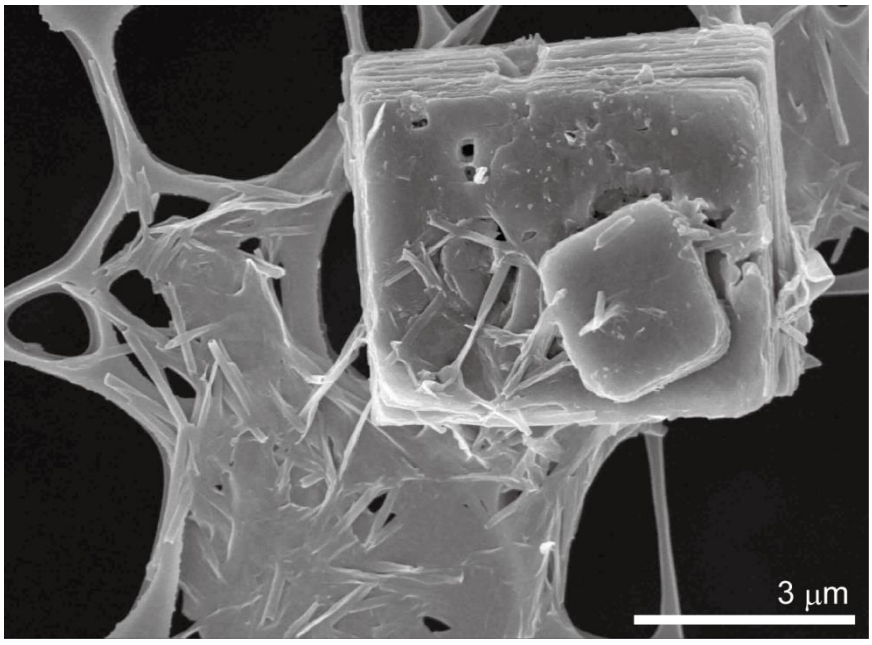

Fig. S3 SEM image of another view of solvo-$(C_{18})_2$DMA-Oct.

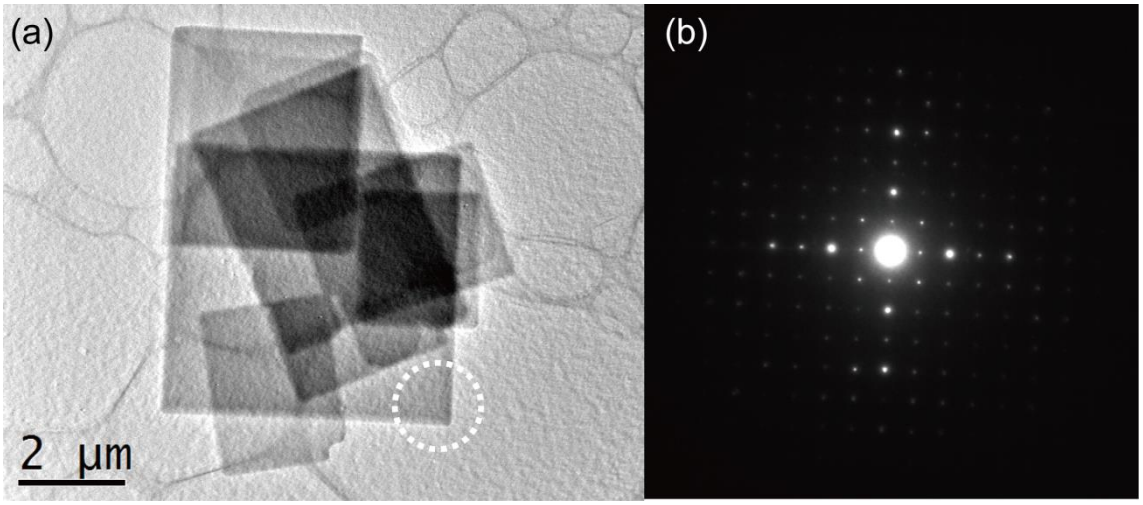

Fig. S4 (a) TEM image of layered octosilicate and (b) ED pattern of the selected circular area, shown by the white dots in the image (a).

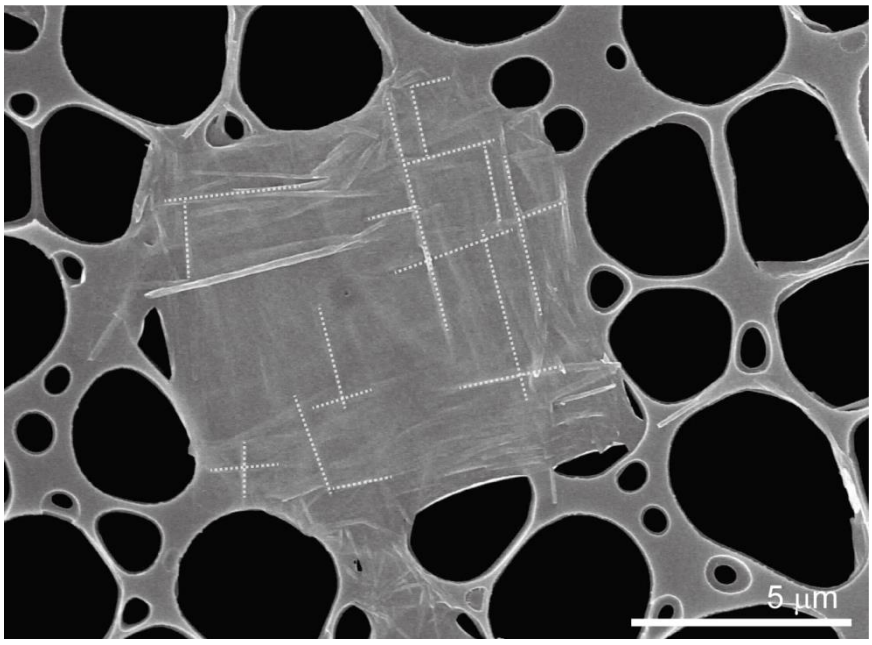

Fig. S5 SEM image of another view of solvo-$(C_{18})_2$DMA-Oct. (The lines shown by the white dots indicate the direction of nanoscrolls.)

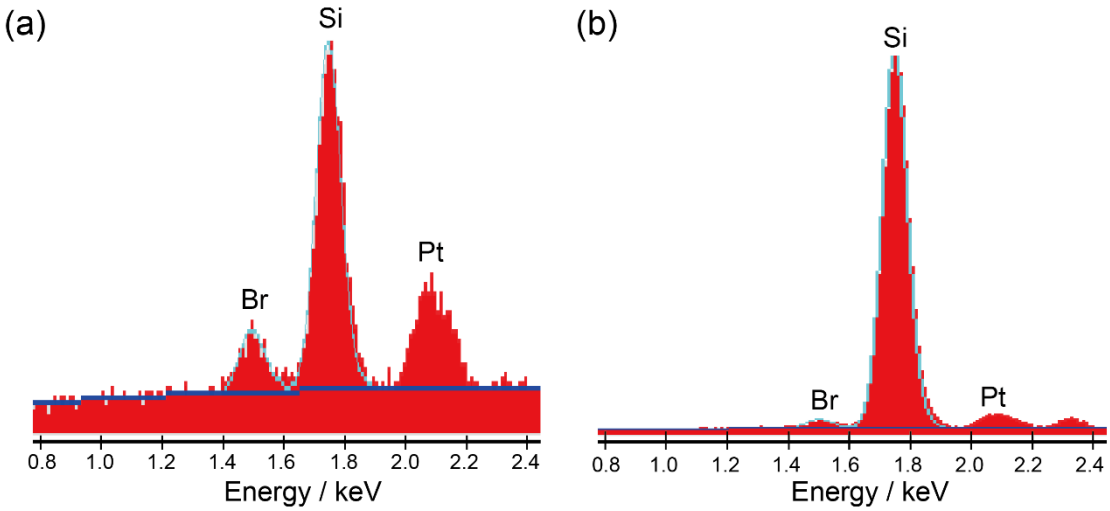

Fig. S6 EDX spectra of (a) $(C_{18})_2$DMA-Oct and (b) solvo-$(C_{18})_2$DMA-Oct.
Pt and Pd (not shown) were added by sputtering onto the samples to avoid charge-up.

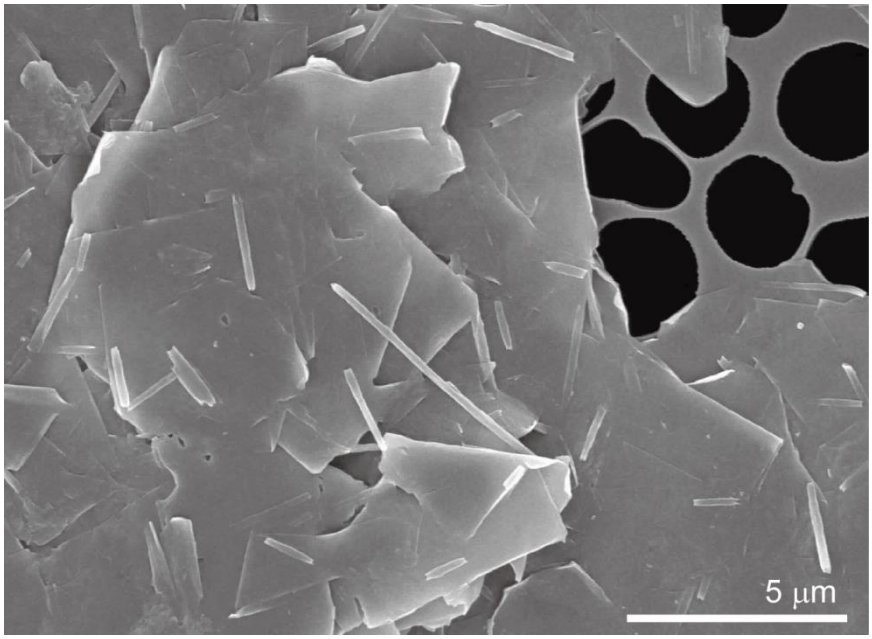

Fig. S7 SEM image of $(C_{18})_2$DMA-Oct heated at 70 °C for 1 d in a Teflon-sealed autoclave.

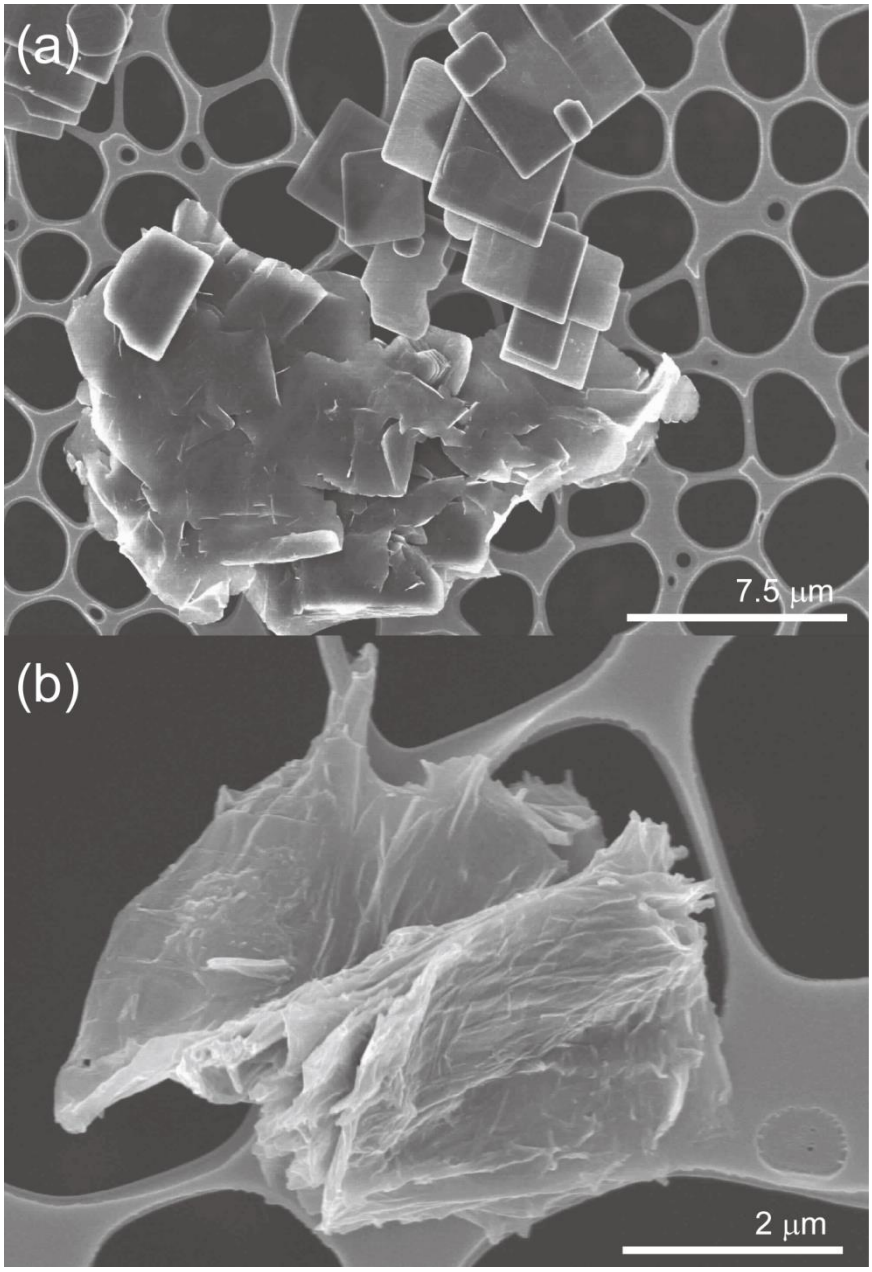

Fig. S8 SEM images of (a) $(C_{18})_2$DMA-Oct heated at 70 °C for 1 d in heptane under stirring with a refluxing condenser and (b) $(C_{18})_2$DMA-Oct treated solvothermally at 120 °C for 1 d in heptane without stirring.