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Structure models for the hydrated and dehydrated nitrate-intercalated layered double hydroxide of Li and Al

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Electronic Supporting Information

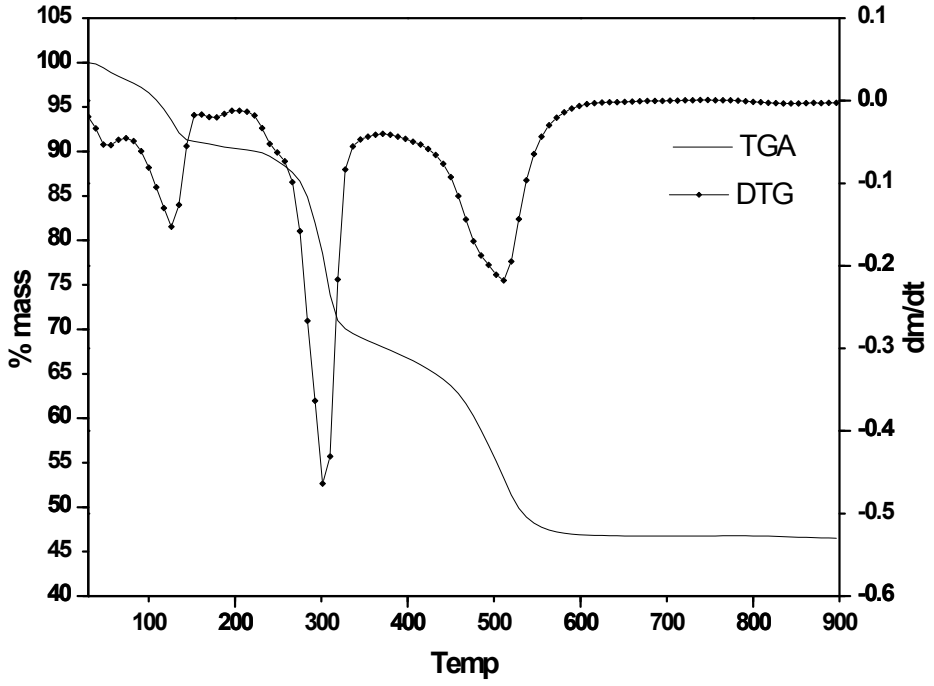

Fig. S1 TGA and DTG curves for the as-prepared [Li-Al-NO_3] (phase I).

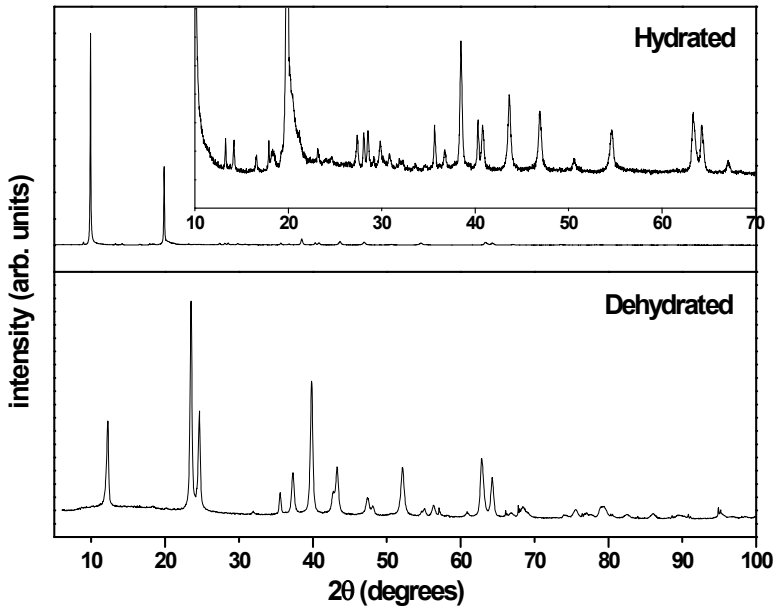

Fig. S2 PXRD pattern of the as-prepared [Li-Al-NO_3] LDH (phase I) compared with that of the dehydrated LDH (phase-II) (50 °C, in vacuo) (data from Russia). Inset shows the data on an expanded intensity scale.

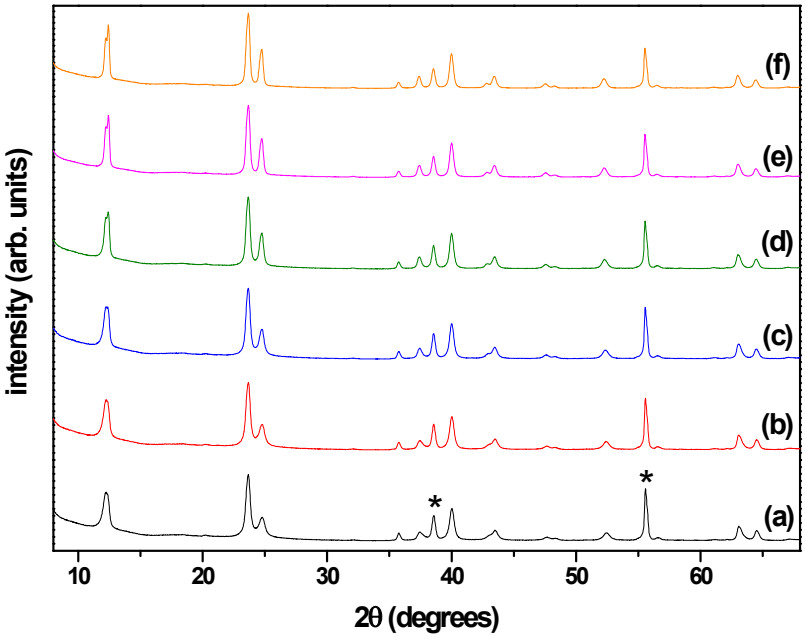

Fig. S3 *In situ* variable temperature PXRD measurements of the dehydrated [Li-Al-NO_3] LDH (phase II) at (a) 30 °C (b) 50 °C (c) 100 °C (d) 150 °C (e) 175 °C (f) 200 °C. Reflections marked by asterisk are due to the Ta strip used as the substrate.

Table S1 Assignment of the prominent observed Bragg reflections* of phase I

	Hexagonal a = 5.08 Å, c = 17.91 Å
2θ [°]*	*hkl*
9.9	*002*
19.9	*004*
35.7	*111*
36.8	*112*
38.5	*113*
40.3	*008*
40.8	*114*
43.6	*115*
46.9	*116*
50.6	*117*
54.6	*118*
63.4	*300*
64.2	*302*
67.1	*217*
73.5	*304*

***** Weak reflections appearing in the range of 11-19 °2θ and 22-35 °2θ are excluded.

Table S2 Refined atomic position parameters of phase I in hexagonal symmetry

Atom type	**Wyckoff position**	***x***	***y***	***z***	**SOF**
O1	12*i*	-0.00438	0.64234	0.05222	1
Al	4*f*	0.33330	0.66670	0.00000	1
Li	2*b*	0.00000	0.00000	0.00000	1
N	6*h*	0.37839	0.01141	0.25000	0.33333
O2	12*i*	0.25144	0.78233	0.19887	0.16667
O3	12*i*	0.19568	0.06039	0.28745	0.16667
O4	12*i*	0.64912	0.10755	0.26987	0.16667
O5	12*i*	0.97566	0.38073	0.30063	0.20249

Table S3 Refined bond lengths and angles of phase I in hexagonal symmetry

Bond distances (Å)	
Al – O1	1.8729, 1.9027
Li – O1	2.0338
N-O2	1.3623
N-O3	1.2664
N-O4	1.2595
O2-O5	2.5647
O3-O5	2.4950
O4-O5	2.6153
Li-O3	3.8991
Al-O2	3.6594
O1-O5	3.2210
Bond angles (°)	
O1-Al-O1	77.979, 86.954
O1-Li-O1	79.382
O2-N-O3	116.228
O2-N-O4	118.650
O3-N-O4	122.770
Non bonded distances (Å)	
In-plane O1 – O1	2.376, 2.598