Supporting information

Synthon Approach to Structure Models for the Bayerite-derived Layered Double Hydroxides of Li and Al

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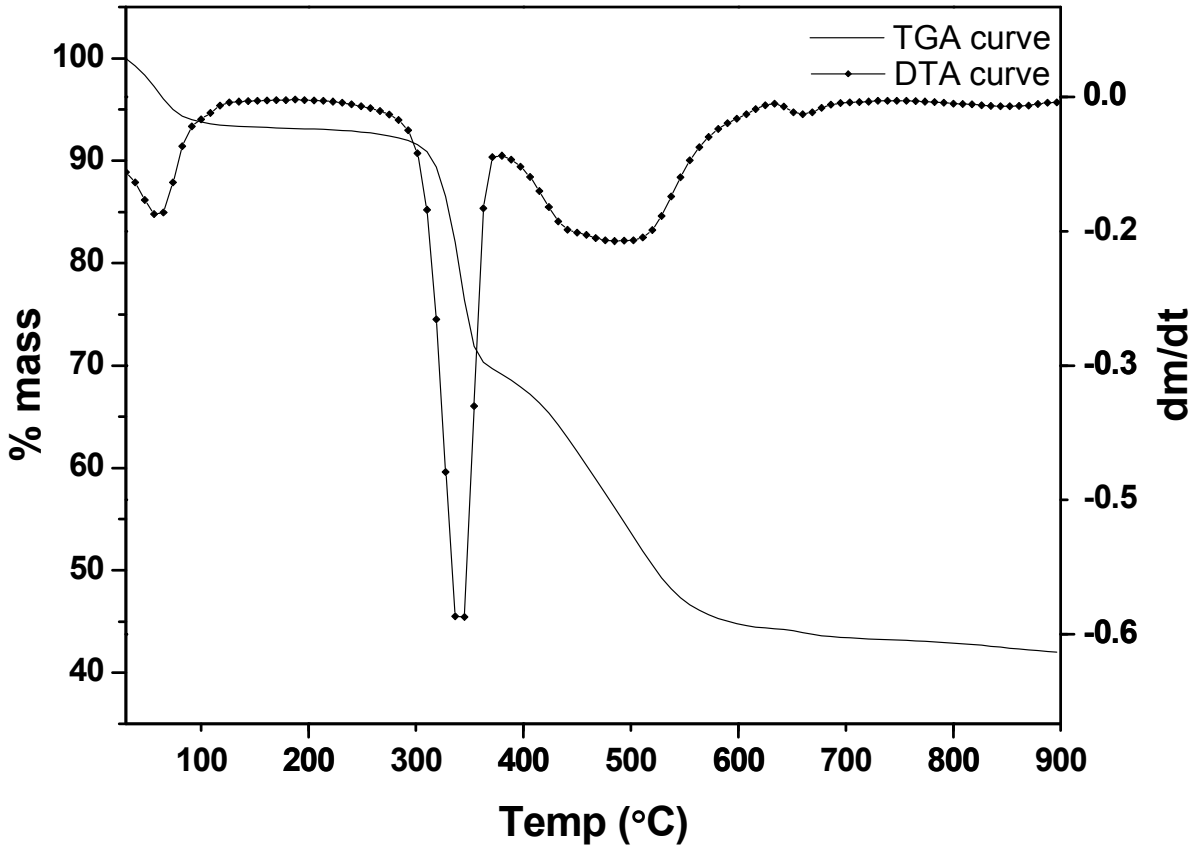

Figure S1. TGA and DTG curve of phase-I LDH. The sample was stayed at 900 °C to constant weight.

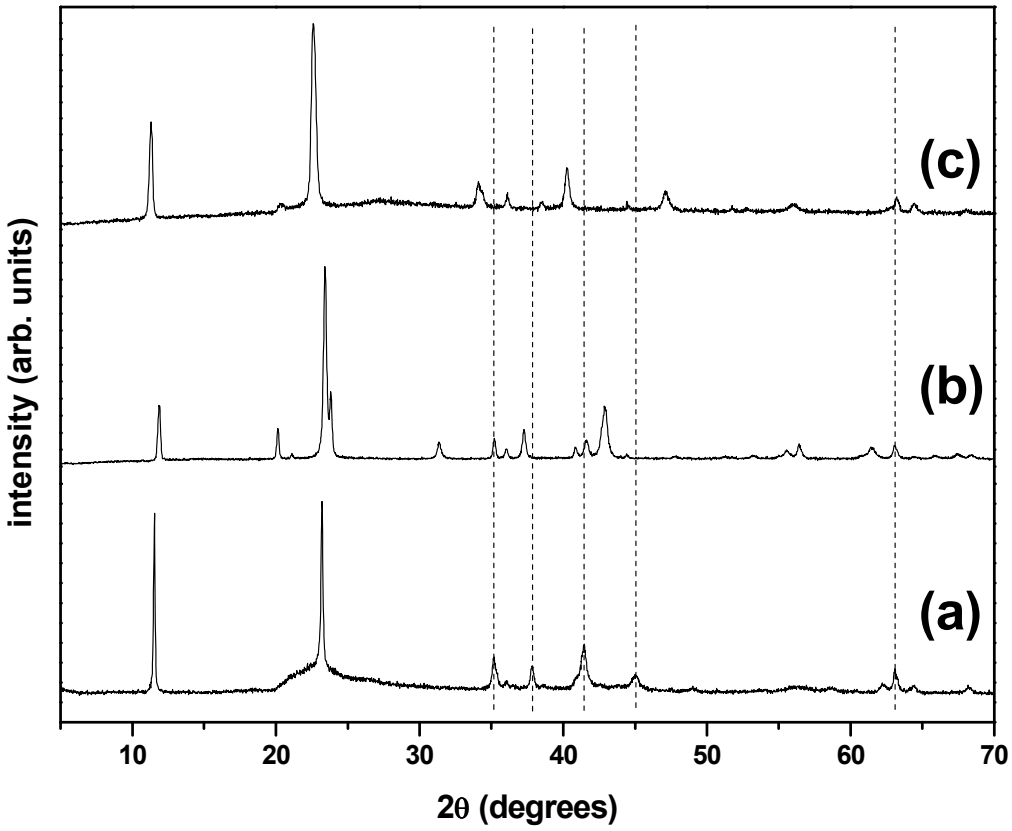

Figure S2. PXRD pattern of the bayerite-derived [Li-Al-Br] LDH: (a) as-prepared, (b) dehydrated at 120 °C, and (c) (b) rehydrated at RH ~ 70%.

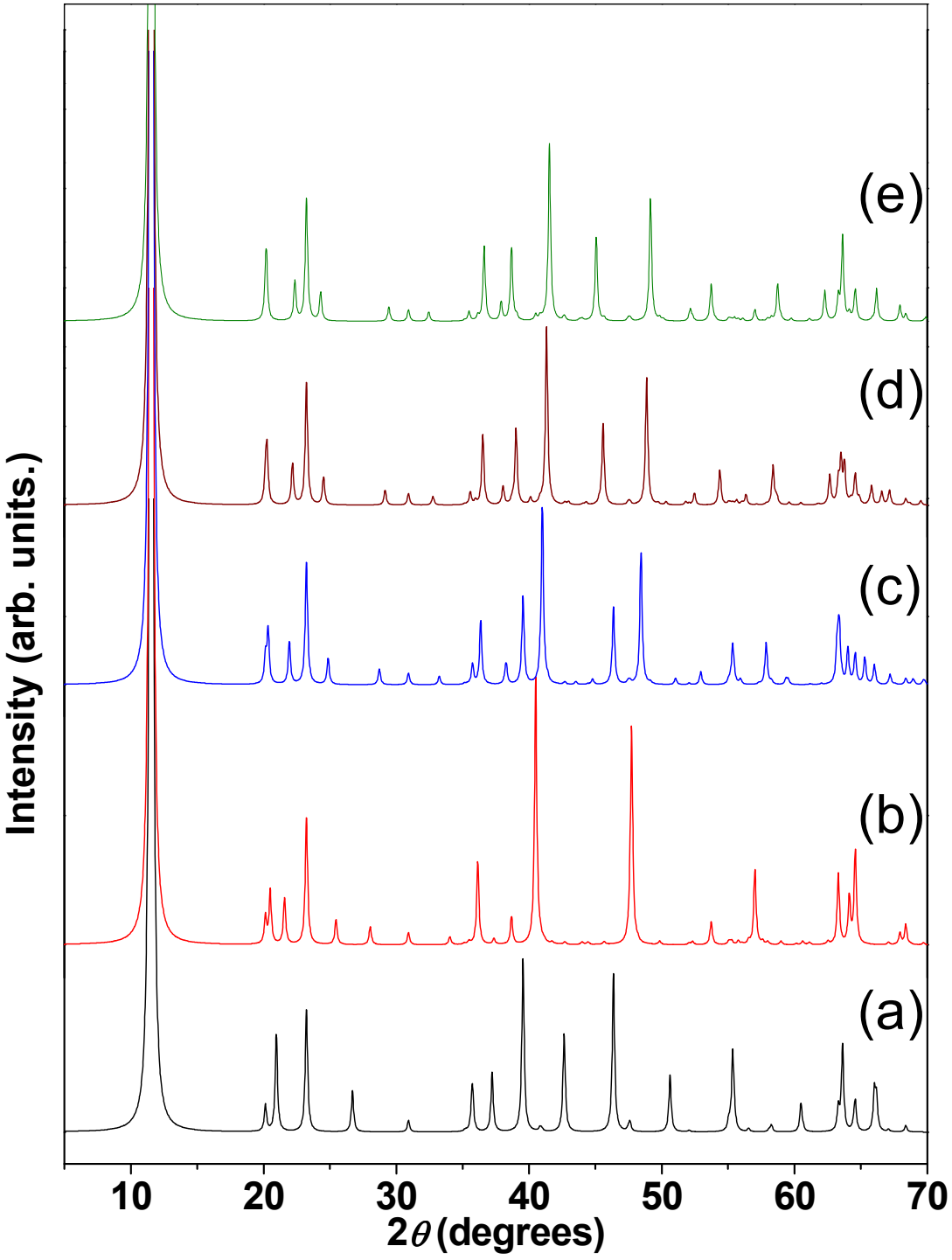

Figure S3. Simulated PXRD pattern for model structures of b-[Li-Al-Br] with stacking vectors (*a*/n, 0, z) (a) n = 2, (b) n = 3, (c) n = 4, (d) n = 5, (e) n = 6.

Table S1. Bond distances and bond angles of phase-I, phase-II and phase-III of b-[Li-Al-Br] LDH obtained from Rietveld refinement

	Phase-I	**Phase-II**	**Phase-III**
Bond distances (Å)			
Al – O1	1.8772 , 1.9080	1.8945	1.9011, 1.9326
Al – O2	1.9490	NA	1.9121
Li – O1	2.0189	2.0953	2.0258
Li – O2	2.0672	NA	2.0845
Al – Br1	3.8237	-	3.9432
Li – Br1	-	3.7566	-
Al – Br2	-	NA	-
Li – Br2	3.8143	NA	3.9762
Al – Ow1	3.8370, 3.8474	NA	-
Li – Ow1	-	NA	-
Al – Ow2	-	NA	-
Li – Ow2	3.8161, 3.8843	NA	-
Br1 – O1	3.2705, 3.3317	3.3638	3.2419, 3.2984
Br2 – O1	3.2332, 3.3743	NA	3.5987, 3.6515
Br1 – O2	3.1231, 3.1899	NA	3.5225, 3.6149
Br2 – O2	3.3556, 3.6843	NA	3.0947, 3.1947
O1 – Ow1	3.2465, 3.2597	NA	2.9941, 3.0194
O1 – Ow2	3.3231, 3.2372	NA	NA
O2 – Ow1	3.1744, 3.1826	NA	3.7677, 3.9159
O2 – Ow2	3.4622, 3.8106	NA	NA
Bond angles (°)			
O1 – Al – O1	81.317, 89.329	77.351, 89.657	80.978, 87.594
O1 – Al – O2	85.905	NA	87.990
O2 – Al – O2	75.949	NA	78.089
O1 – Li – O1	81.631	78.200	82.643
O1 – Li – O2	80.058	NA	80.226