

Supporting Information:

Direct Molecular Confinement in Layered Double Hydroxides: From Fundamentals to Advanced Photo-luminescent Hybrid Materials

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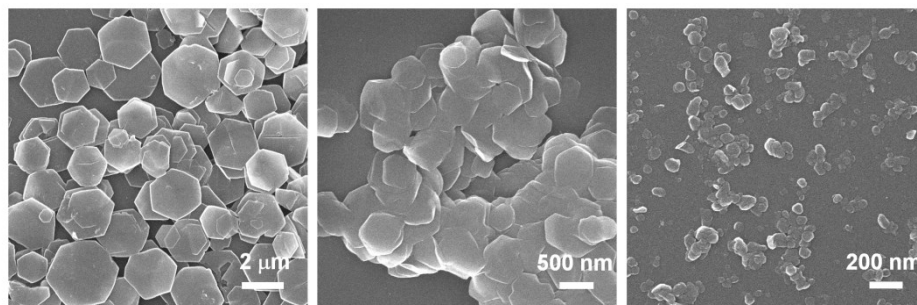


Fig. S1 The SEM images of as-prepared Mg₂Al-L (left), Mg₂Al-M (mid), and Mg₂Al-S (right).

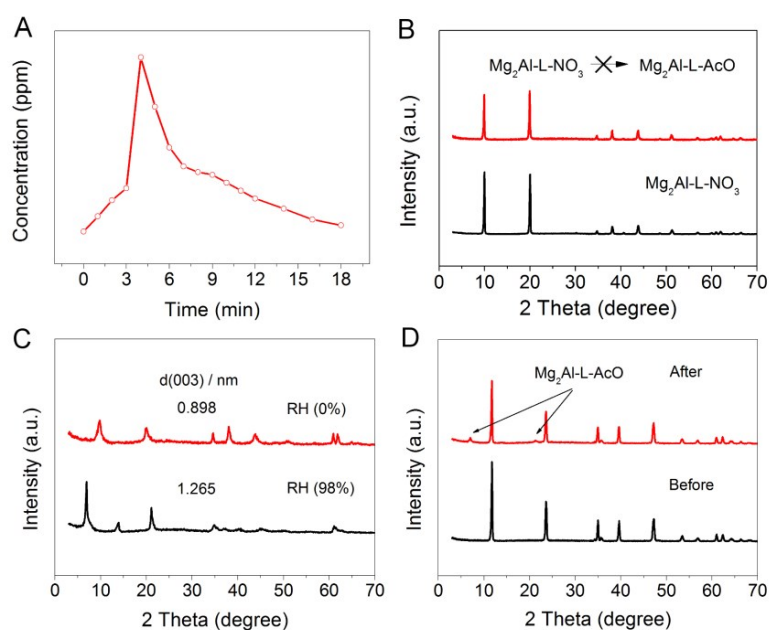


Fig. S2 A) The concentration curve of CO₂ during acetates intercalation reaction, B) the powder XRD patterns of Mg₂Al-L-NO₃ before and after reaction, C) the powder XRD patterns of Mg₂Al-L-AcO at different relative humidity (RH), and D) the powder XRD patterns of Mg₂Al-L before and after reaction in water.

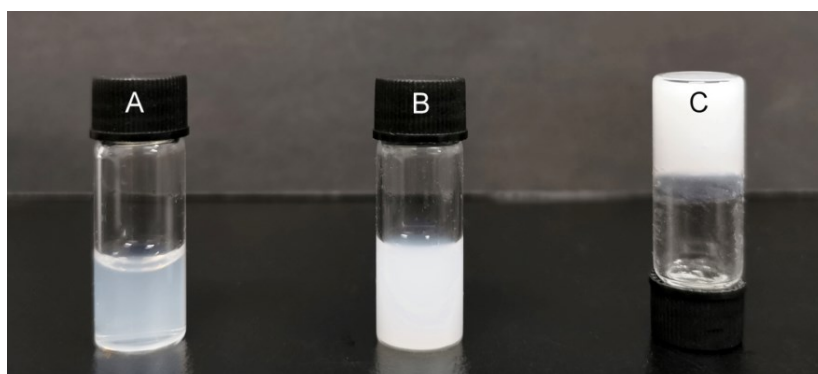


Fig. S3 The photographs of Mg₂Al-M-AcO in water at different concentrations: A) $c = 1 \text{ mg mL}^{-1}$, B) $c = 10 \text{ mg mL}^{-1}$, and C) $c = 20 \text{ mg mL}^{-1}$.

Table S1. The experimental parameters and yields of the intercalation reactions.

	LDHs	Organic acid	pKa	<i>n</i> (mmol)	<i>V</i> or <i>m</i>	Yield	
The direct method	Mg ₂ Al-L			2.463	141 μL	103 mg 92.03 %	
	Mg ₂ Al-M			1.231	71 μL	94 mg 83.54 %	
	Mg ₂ Al-S			1.026	59 μL	88 mg 78.62 %	
	Zn ₂ Al-L	Acetic acid	4.76	1.642	78 μL	76 mg 52.19 %	
	Ni ₂ Fe-L			3.284	188 μL	80 mg 52.63 %	
	Co ₂ Al-L			1.642	78 μL	93 mg 66.27 %	
	Tris-LDH			0.616	35 μL	96 mg 83.70 %	
			Chloroacetic acid	2.86	2.463	147 μL	105 mg 83.29 %
			Dichloroacetic acid	1.30	2.463	203 μL	125 mg 89.16 %
			Propionic acid	4.87	3.284	245 μL	105 mg 89.22 %
			Acrylic acid	4.26	2.463	169 μL	98 mg 83.84 %
		Mg ₂ Al-L	<i>p</i> -Fluorobenzoic acid	4.14	2.873	403 mg	127 mg 87.71 %
			<i>p</i> -Toluic acid	4.35	2.873	391 mg	104 mg 72.64 %
			<i>p</i> -Nitrobenzoic acid	3.44	2.873	480 mg	120 mg 76.98 %
			<i>p</i> -Hydroxybenzoic acid	4.48	2.873	397 mg	100 mg 69.46 %
		<i>p</i> -phthalic acid	3.54	1.231	205 mg	106 mg 87.33 %	
The stepwise method							
			Trichloroacetic acid	0.70	2.586	259 μL	134 mg 86.82 %
			Glycolic acid	3.83	2.586	197 mg	106 mg 89.79 %
			Lactic acid	3.86	3.284	245 μL	114 mg 91.98 %
			Oxalic acid	1.27	3.284	296 mg	92 mg 86.66 %
			Propanedioic acid	2.85	3.284	342 mg	97 mg 88.77 %
			Succinic Acid	4.19	3.284	388 mg	99 mg 88.10 %
			Benzoic Acid	4.20	3.284	401 mg	117 mg 85.15 %
			Methanesulfonic acid	-1.92	0.821	53 μL	110 mg 86.80 %
			Ethanesulfonic acid	-1.68	1.231	136 mg	70 mg 52.84 %
			Isethionic acid	-1.60	0.739	93 mg	111 mg 79.83 %
		Mg ₂ Al-L	2-Acrylamido-2-methylpropane sulfonic acid	--	1.231	255 mg	140 mg 81.22 %
			<i>p</i> -Toluenesulfonic acid	-2.80	1.231	234 mg	124 mg 78.50 %
			1,2-Ethanedisulfonic acid	--	0.616	117 mg	100 mg 60.48 %
			1,5-Naphthalenedisulfonic acid	--	1.642	473 mg	120 mg 58.36 %
		Methylenediphosphonic acid	--	0.739	130 mg	97 mg 78.61 %	
		Phenylphosphonic acid	--	1.642	260 mg	110 mg 72.29 %	
		TPE carboxylic acid	--	0.821	309 mg	185 mg 76.51 %	

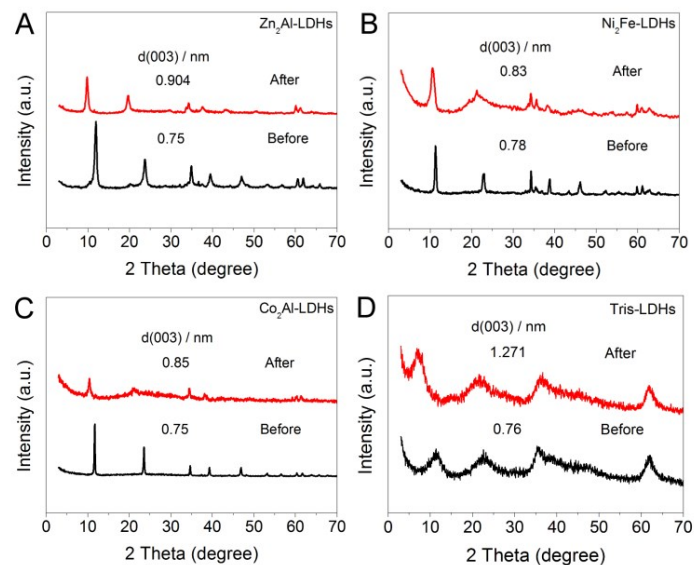


Fig. S4 The powder XRD of A) Zn₂Al-LDHs, B) Ni₂Fe-LDHs, C) Co₂Al-LDHs, and D) Tris-LDHs before and after acetate intercalation.

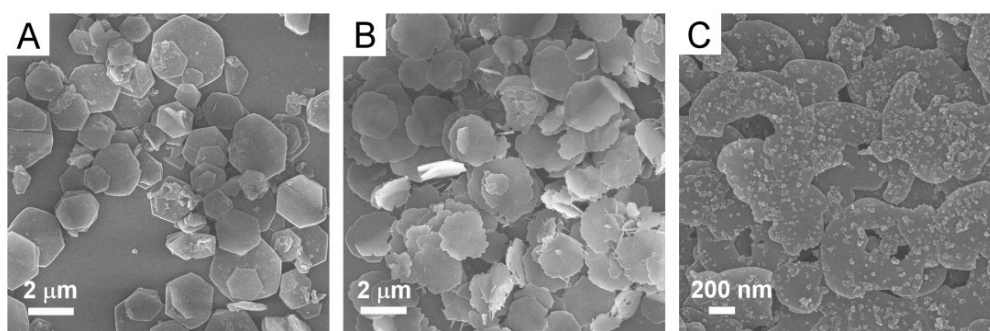


Fig. S5 The SEM images of A) Zn₂Al-LDHs, B) Ni₂Fe-LDHs, C) Co₂Al-LDHs after acetate intercalation.

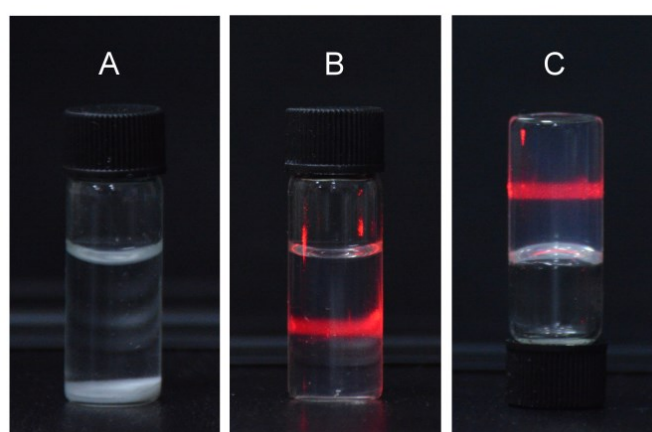


Fig. S6 The photographs of A) Tris-LDHs dispersed in water (*c*: 10 mg mL⁻¹), B) Tris-LDHs-AcO in water (*c*: 10 mg mL⁻¹), and C) the gel state of Tris-LDHs-AcO in water (*c*: 25 mg mL⁻¹).

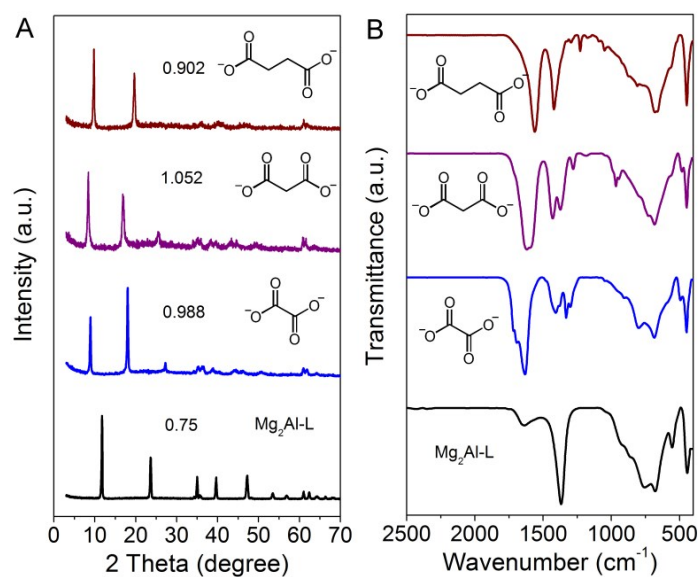


Fig. S7 A) The powder XRD and B) the FT-IR of Mg_2Al-L intercalated with different aliphatic dicarboxylates.

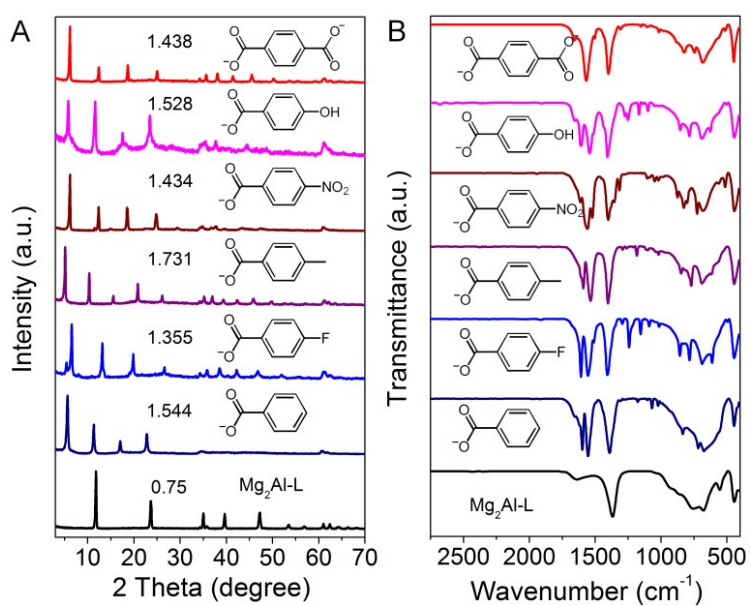


Fig. S8 A) The powder XRD and B) the FT-IR of Mg_2Al-L intercalated with different aromatic carboxylates.

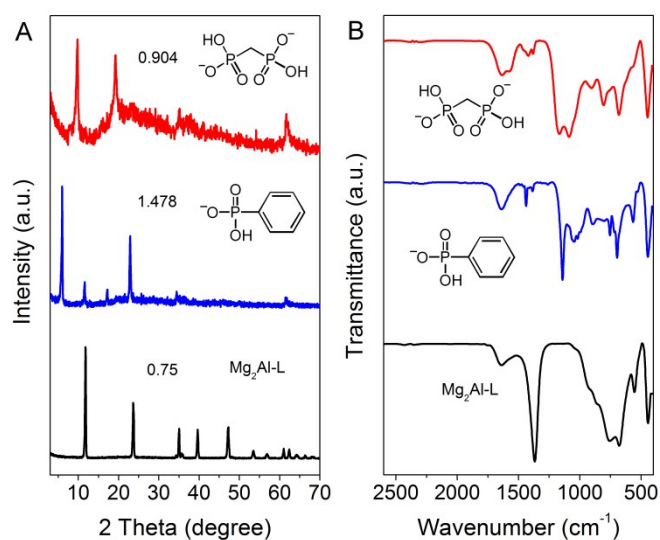


Fig. S9 A) The powder XRD and B) the FT-IR of $\text{Mg}_2\text{Al-L}$ intercalated with different phosphonates.

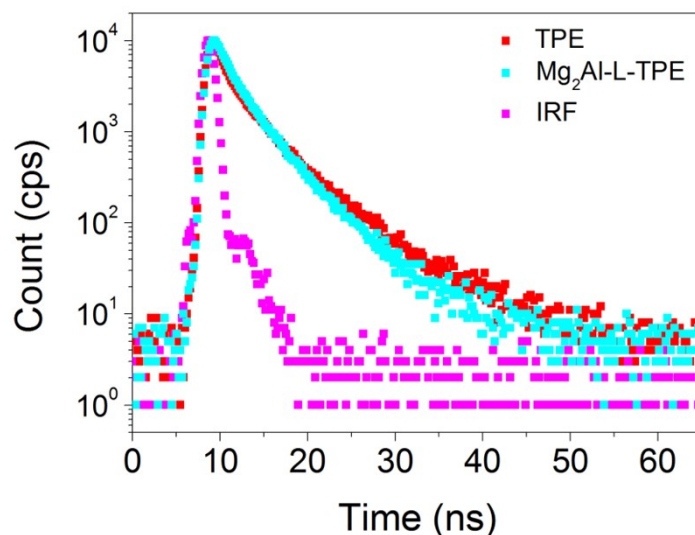


Fig. S10 The fluorescence decay curves of TPE carboxylates and the $\text{Mg}_2\text{Al-L-TPE}$ hybrid, where the lifetime τ is obtained by fitting the equation $I_t = I_0 + B_1 \cdot \exp(-t/\tau_1) + B_2 \cdot \exp(-t/\tau_2)$, and $\tau = B_1 \cdot \tau_1^2 + B_2 \cdot \tau_2^2 / (B_1 \cdot \tau_1 + B_2 \cdot \tau_2)$.

Table S2. The fluorescence lift time and absolute quantum yield of TPE carboxylates and the $\text{Mg}_2\text{Al-L-TPE}$ hybrid.

	Life time (ns)						Quantum yield (%)
	I_0	B_1	B_2	τ_1	τ_2	τ	
TPE carboxylates	1.804	0.239	0.046	1.42	5.41	3.10	16.88
$\text{Mg}_2\text{Al-L-TPE}$	2.017	0.183	0.047	1.72	4.68	2.94	23.72