Supporting Information

Dual modification of LiNi_{0.6}Co_{0.2}Mn_{0.2}O₂ with MgHPO₄ as a high-performance cathode material for Li-ion batteries

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Fig. S1 Rietveld refinements from the XRD patterns of (a) LMR@MgHP-1 and (b) LMR@MgHP-5.

Table S1. Rietveld refinement results of LMR@MgHP-1 X-ray powder diffraction based on different possible models.

Hypothetical	Location of	Reliability factors / %				
models	Mg atoms	R _p	R _{wp}	Bragg R-	RF-factor	
				factor		
No.1	Nowhere	6.46	8.15	6.46	4.01	
No.2	Li layer	6.20	7.87	5.97	3.57	
No.3	TM layer	6.49	8.35	6.54	3.94	
No.4	Dual sites	6.48	8.34	6.53	3.94	

Table S2. Rietveld refinement results of LMR@MgHP-2 X-ray powder diffraction based on different possible models.

Hypothetical	Location of	ity factors / %	factors / %		
models	Mg atoms	R _p	R_{wp}	Bragg R- factor	RF-factor
No.1	Nowhere	6.67	8.59	6.10	3.65

No.2	Li layer	6.57	8.42	6.01	3.51
No.3	TM layer	6.72	8.69	8.69	3.73
No.4	Dual sites	6.69	8.66	6.12	3.65

 Table S3. Rietveld refinement results of LMR@MgHP-5 X-ray powder diffraction based on different possible models.

Hypothetical	Location of	Reliability factors / %				
models	Mg atoms	R _p	\mathbf{R}_{wp}	Bragg R-	RF-factor	
				factor		
No.1	Nowhere	6.70	8.79	6.24	3.98	
No.2	Li layer	6.51	8.57	6.21	3.82	
No.3	Ni layer	6.75	8.88	6.30	4.04	
No.4	Dual sites	6.88	9.00	6.60	4.19	

Table. S4 EDX analysis results of LMR@MgHP-2 sample.

Element	Ni K	Co K	Mn K	Mg K	P K	O K
Wt%	41.50	13.92	13.12	0.35	0.57	30.54
At%	22.65	7.57	7.65	0.47	0.53	61.13



Fig. S2 The variations in the atomic concentration of Mg element as a function of depth for LMR@MgHP-2 sample.



Fig. S3 P 2p spectra for LMR@MgHP-2 sample.



Fig. S4 The initial charge-discharge profiles at 0.1C between 2.8 and 4.3 V for all the samples.



Fig. S5 Average discharge potential of LMR and LMR@MgHP-2 at 1C.