Supplementary information

Improving the structural stability and electrochemical performance of $Na_2Li_2Ti_6O_{14}$ particles via MgF_2 coating

Wei-Wei Ma [a], Hai-Tao Yu [a], Chen-Feng Guo [a], Ying Xie [a,*], Ning Ren [b,*], Ting-Feng Yi [c,*],

[a] Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, School of Chemistry and Materials Science, Heilongjiang University, Harbin, 150080, PR China

[b] Zhejiang Chilwee Chuangyuan Industry Co., Ltd, Changxing, Zhejiang 313100, PR China

[c] School of Resources and Materials, Northeastern University at Qinhuangdao, Qinhuangdao, 066004, PR China

*Corresponding author: Ying Xie

E-mail: xieying@hlju.edu.cn (Dr. Ying Xie).

*Corresponding author: Ning Ren

Email: rnrm040412@163.com (N. Ren);

*Corresponding author: Ting-Feng Yi

E-mail: tfyihit@163.com (Dr. Ting-Feng Yi).

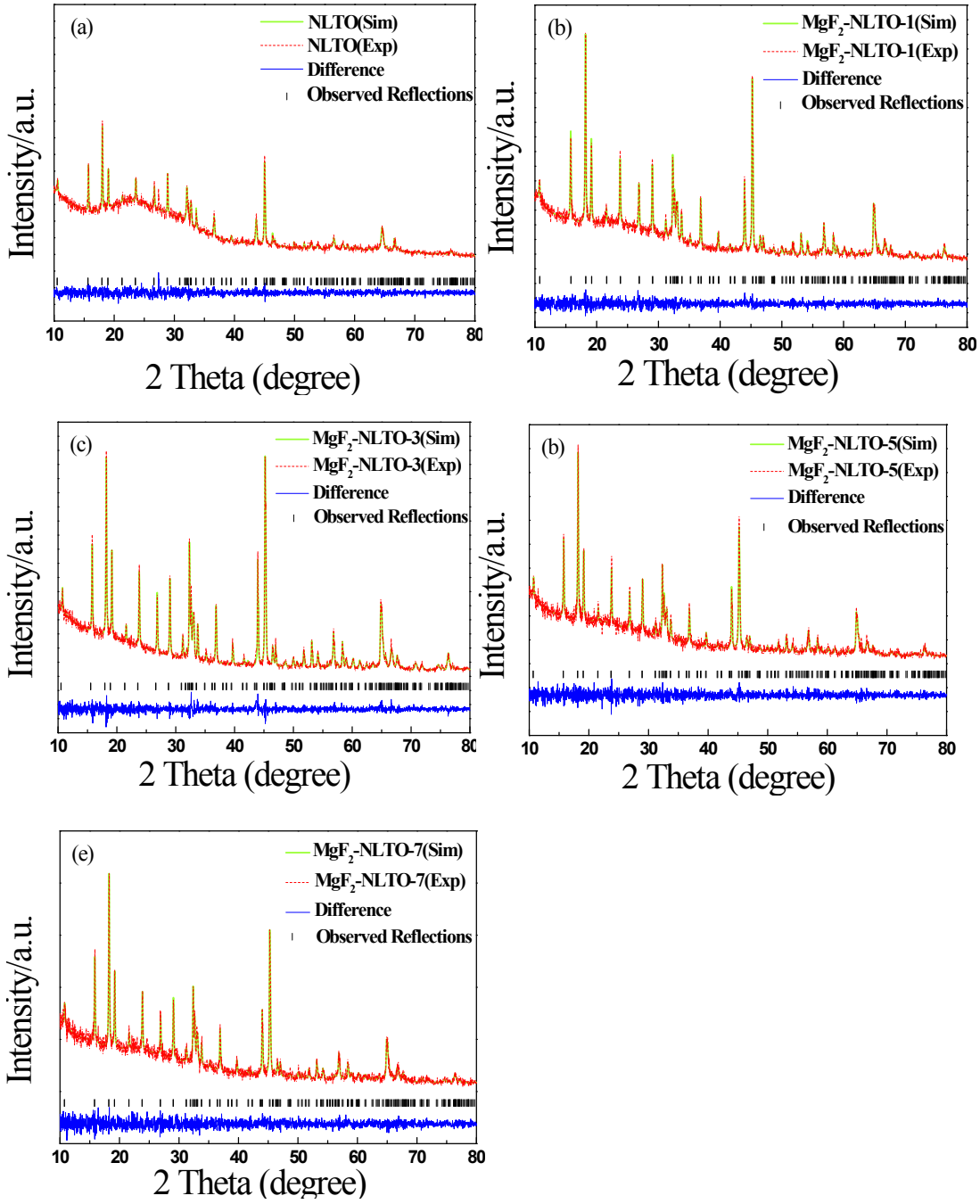

Fig. S1 Reitveld refinements for (a) NLTO, (b) MgF_2-NLTO-1, (c) MgF_2-NLTO-3, (d) MgF_2-NLTO-5, and (e) MgF_2-NLTO-7 samples.

Table S1 Lattice constants (Å), volumes, and relevant $R_{wp.}$ calculated from Rietveld refinement for different samples.

	NLTO	MgF_2-NLTO-1	MgF_2-NLTO-3	MgF_2-NLTO-5	MgF_2-NLTO-7
a (Å)	5.737	5.734	5.741	5.739	5.769
b (Å)	11.2245	11.226	11.226	11.21	11.221
c (Å)	16.485	16.475	16.459	16.471	16.521
Volume ($Å^3$)	1061.503	1060.463	1060.757	1060.171	1069.359
R_{wp}	5.6%	10.9%	9.5%	8.3%	11.3%
$(V_{mf}-V)/V(\%)$ [a]	0.02%	0.11%	0.09%	0.10%	0.66%

[a] The volume of NLTO is taken as the reference

Table S2 Potentials of the redox peaks (V) and the potential differences between the oxidation and reduction peaks (V) [a] for different samples.

Cycle number	Redox-potention (V)(*a*)		
	1st	2nd	3rd
NLTO	1.43/1.21 (0.22)	1.42/1.17 (0.25)	1.44/1.15 (0.29)
MgF_2-NLTO-1	1.33/1.21 (0.12)	1.35/1.19 (0.16)	1.35/1.21 (0.14)
MgF_2-NLTO-3	1.32/1.22 (0.10)	1.32/1.21 (0.11)	1.32/1.21 (0.11)
MgF_2-NLTO-5	1.35/1.27 (0.08)	1.36/1.27 (0.09)	1.35/1.27 (0.08)
MgF_2-NLTO-7	1.38/1.18 (0.20)	1.36/1.17 (0.19)	1.30/1.14 (0.16)

[a] The values in bracket are the potential difference between the oxidation and reduction peaks

Table S3 Warburg factors and lithium diffusion coefficients for pristine and MgF_2-NLTO samples

Sample	σ ($\Omega\ s^{-0.5}$)	D_{Li} ($cm^2\ s^{-1}$)
NLTO	1471.14	3.53×10^{-17}
MgF_2-NLTO-1	938.57	8.67×10^{-17}
MgF_2-NLTO-3	655.30	1.78×10^{-16}
MgF_2-NLTO-5	554.11	2.49×10^{-16}
MgF_2-NLTO-7	1439.41	3.69×10^{-17}