

Supporting Information

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Double Perovskite $\text{La}_2\text{MnNiO}_6$ as a High-Performance Anode for Lithium-Ion Batteries

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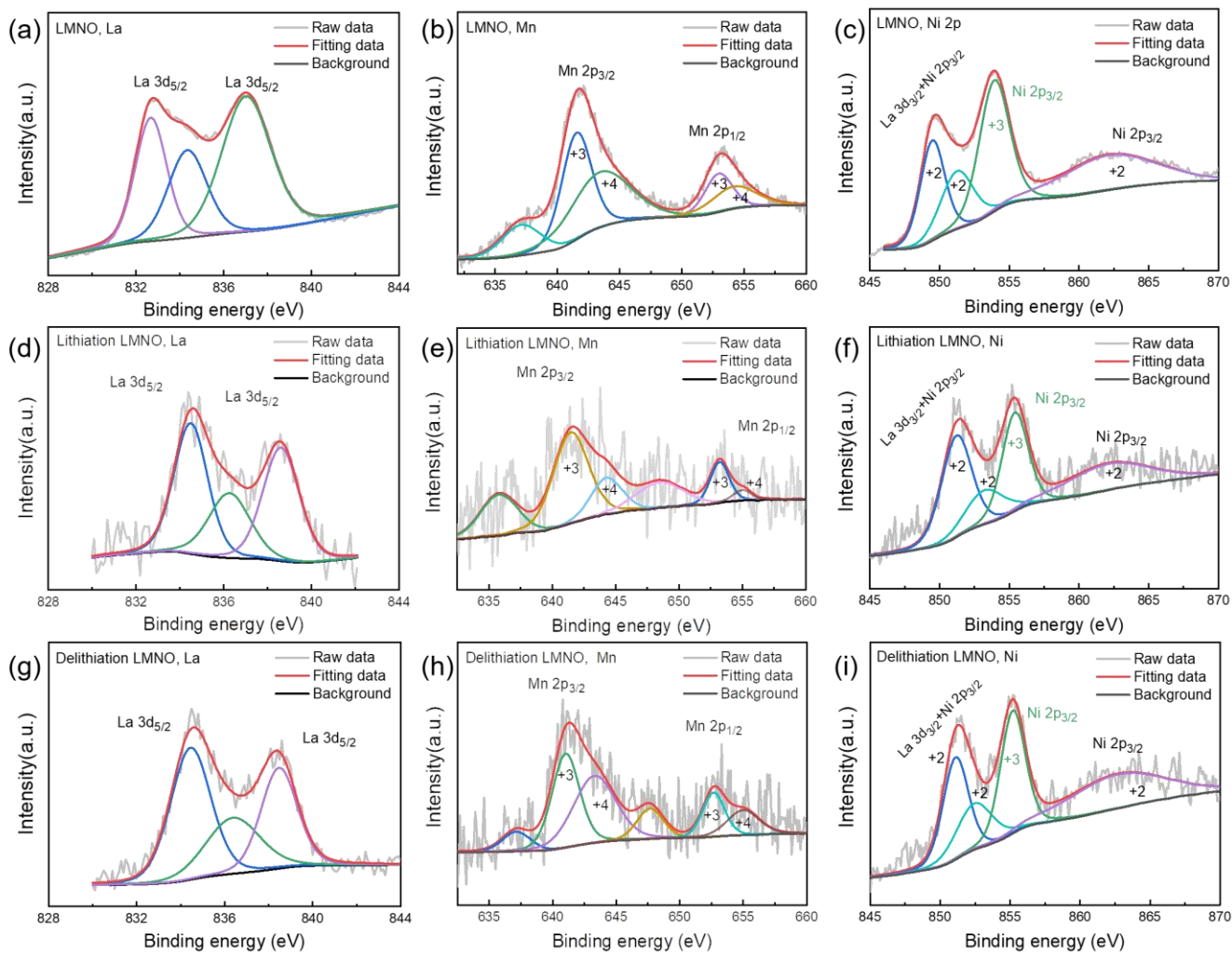


Figure S1. XPS analysis of samples. XPS spectrum of La 3d, Mn 2p and Ni 2p region of LMNO (a-c), lithiation-LMNO (d-f) and delithiation-LMNO (g-i), respectively.

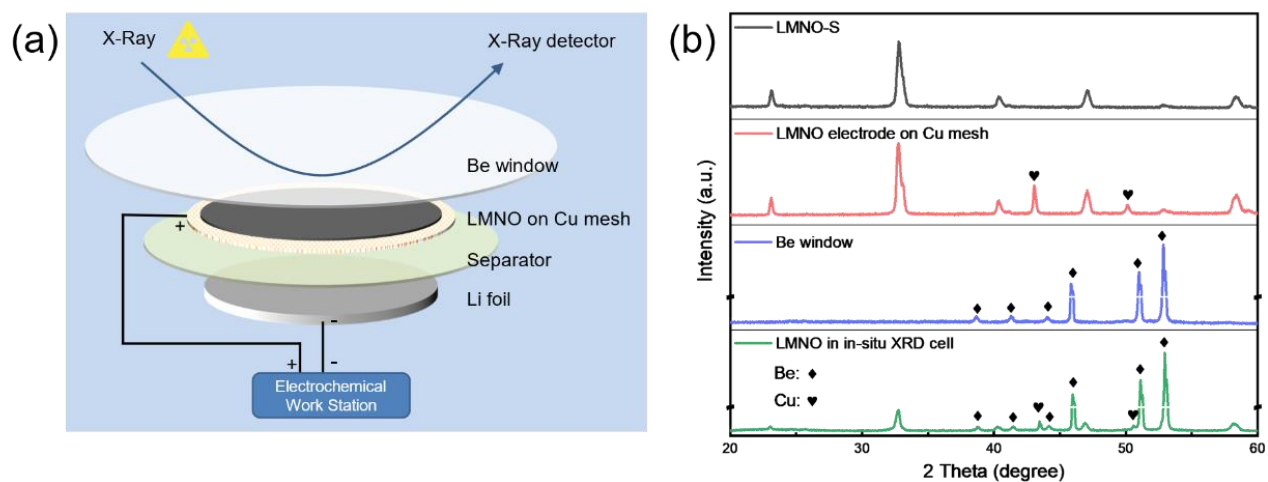


Figure S2.(a) Schematic illustration of in-situ XRD cell. (b) XRD patterns of LMNO-S powder, LMNO electrode, Be window and LMNO electrode in in-situ XRD cell.

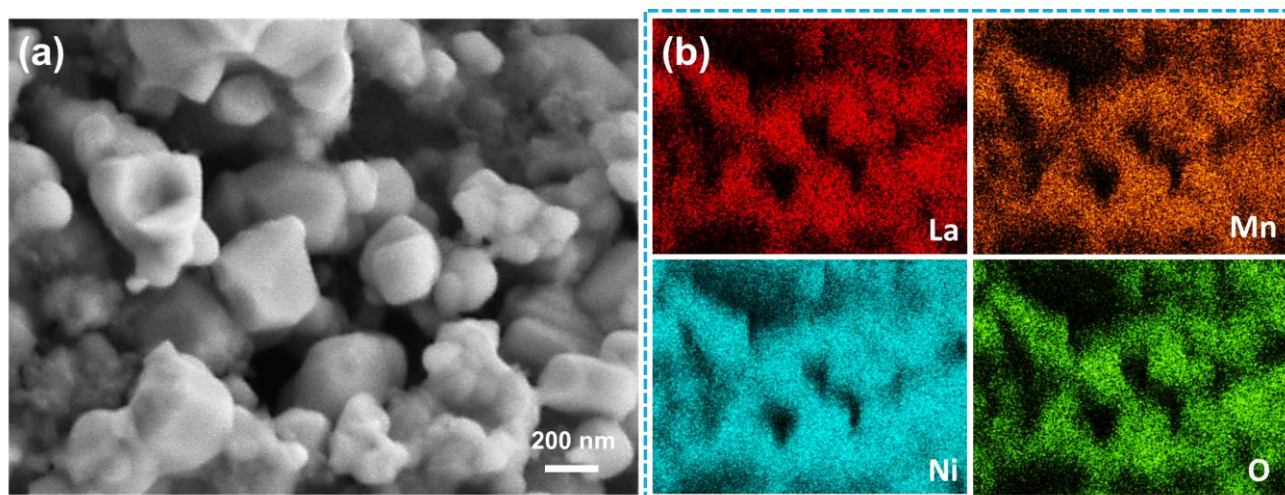


Figure S3.SEM image of LMNO-S and corresponding EDS elemental mapping images of La, Mn, Ni and O elements.

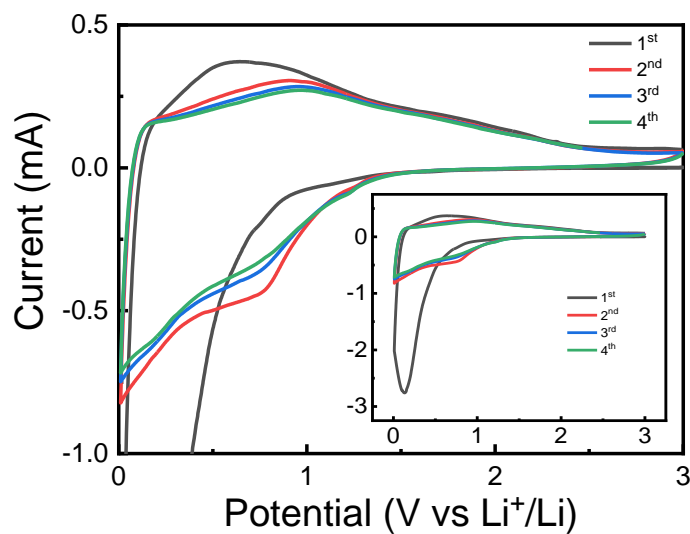


Figure S4. Cyclic voltammograms of Li|LMNO cell with a potential range of 0.01-3.0 V.

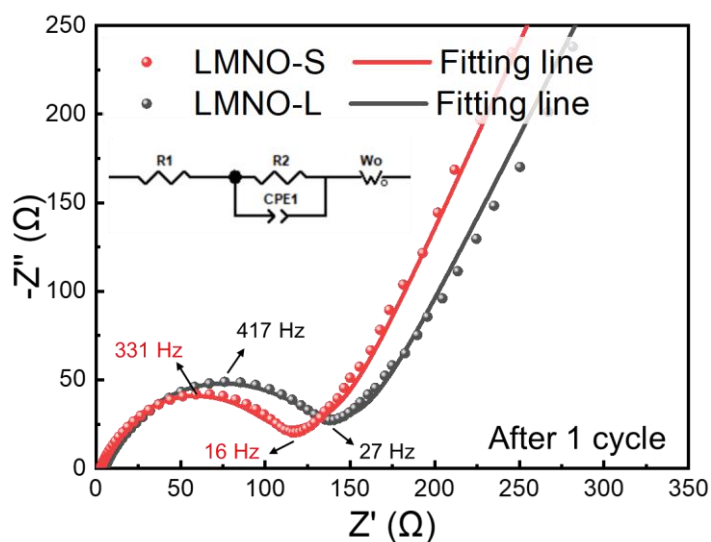


Figure S5. Nyquist plots of LMNO-S and LMNO-L after 1 cycle, the inset is equivalent circuit.

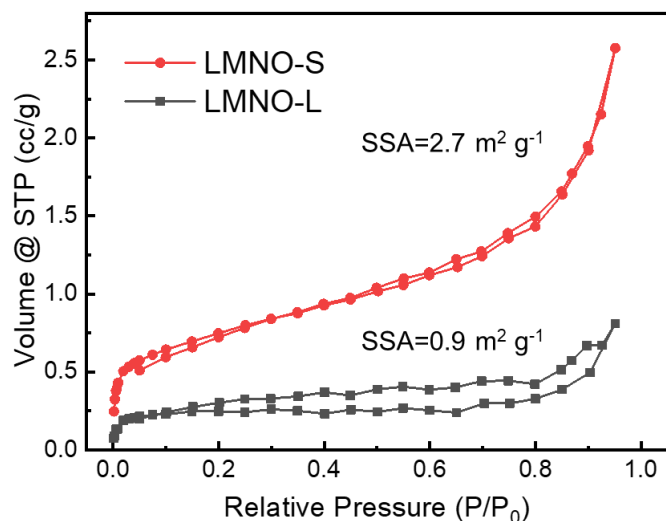


Figure S6. N_2 adsorption and desorption isotherms of LMNO-S and LMNO-L.

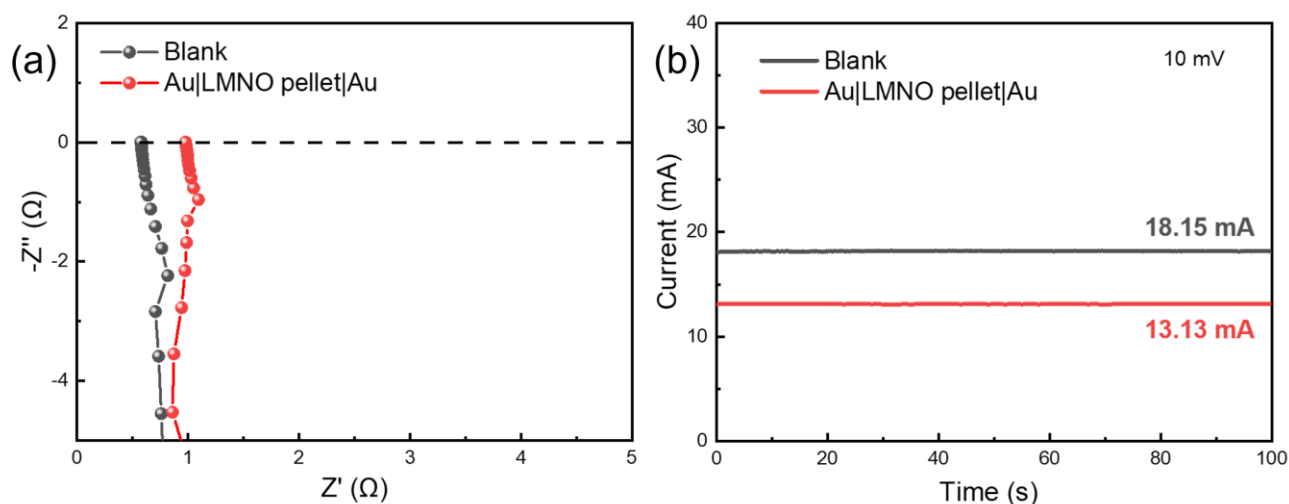


Figure S7. (a), Nyquist plots of LMNO-S pellet. (b), Direct current polarization plots of LMNO-S pellet at 10 mV.

The LMNO fine powder was transferred into a stainless-steel die and pressed, and then the green pellets were sintered at high temperature. The diameter and thickness of LMNO pellet are $d=1.1$ cm and $L=0.1$ cm. EIS result represents that the LMNO-S pellet sample is the good electronic conductor. Direct current polarization data reveal that the ohm resistance of LMNO-S is 0.21Ω . Hence, the

electronic conductivity σ_e is calculated as 0.50 S cm^{-1} according to equation S2, much higher than ionic conductivity of liquid electrolyte in cell ($10^{-2}\sim 10^{-3} \text{ S cm}^{-1}$).

$$R = \rho \frac{L}{S} \quad (\text{S1})$$

$$\sigma_e = \frac{1}{\rho} = \frac{L}{RS} = \frac{4L}{R\pi d^2} \quad (\text{S2})$$

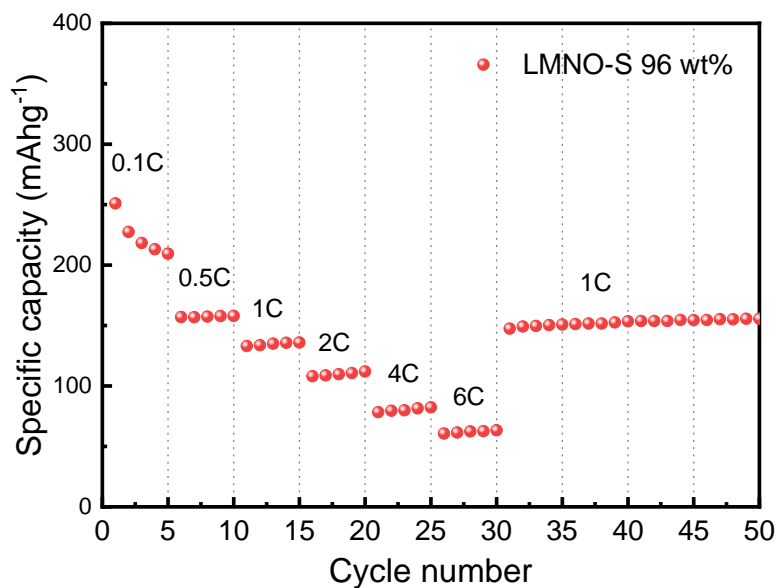


Figure S8. Rate capability of LMNO-S|Li half-cell, in which percent of active material is 96%.

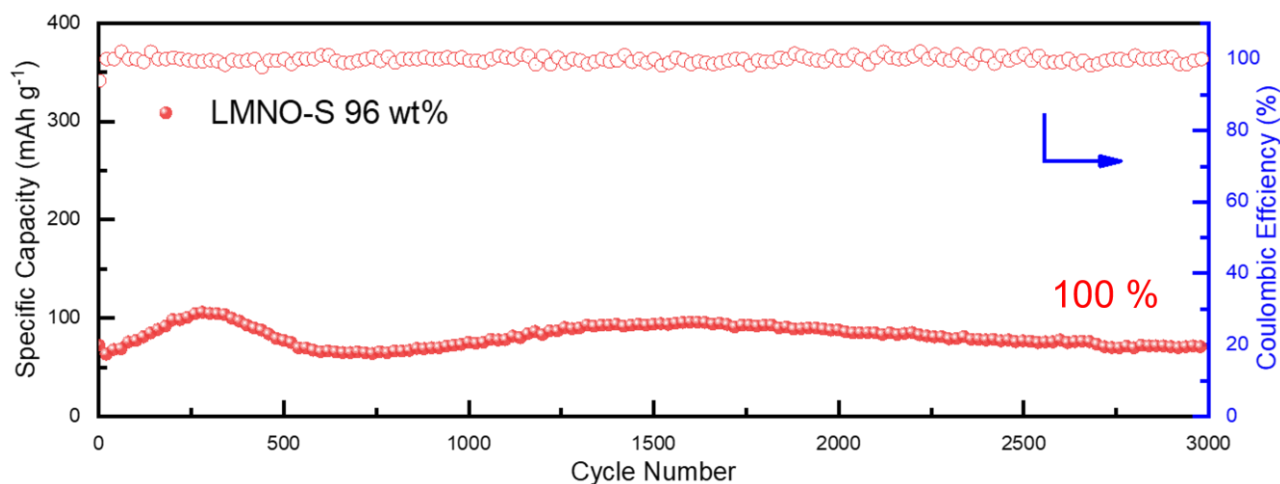


Figure S9. Long cycle performance of LMNO-S|Li half-cell at 6C, in which percent of active material is 96%.

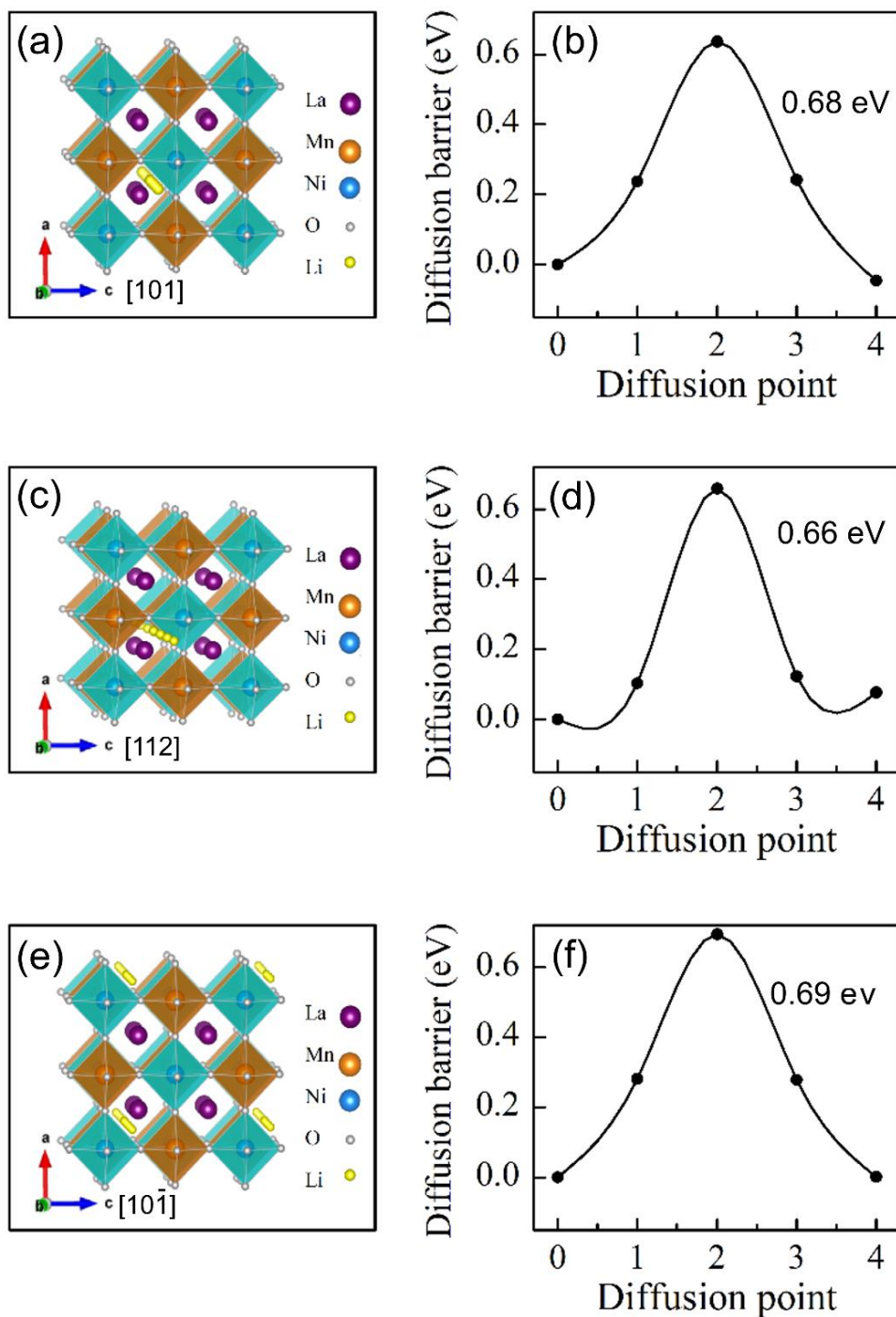


Figure S10. (a) LMNO crystal structure and the Li⁺ diffusion path along [101]. (b) Li diffusion energy along [101]. (c) LMNO crystal structure and the Li⁺ diffusion path along [112]. (d) Li diffusion energy along [112]. (e) LMNO crystal structure and the Li⁺ diffusion path along [10 $\bar{1}$]. (f) Li diffusion energy along [10 $\bar{1}$].

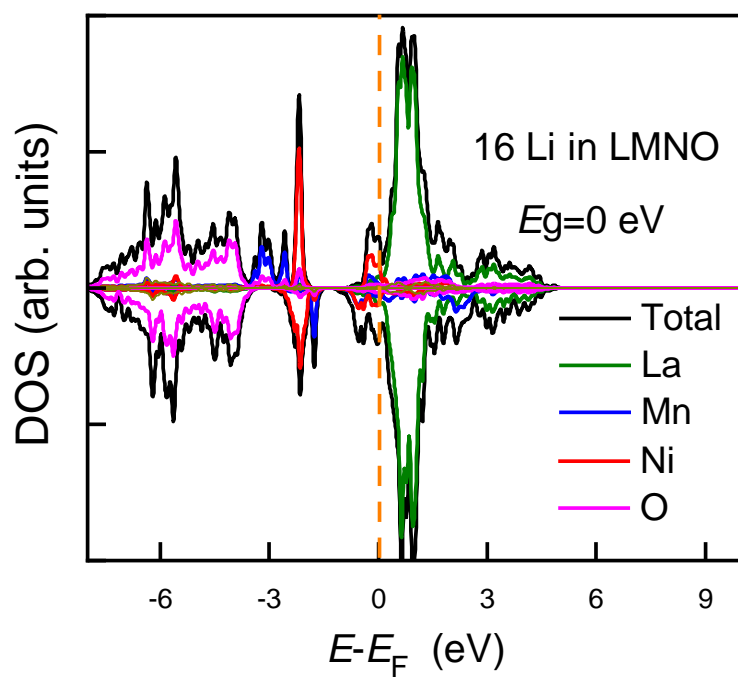


Figure S11. PDOS of Li fully intercalated LMNO.