Supporting Information for

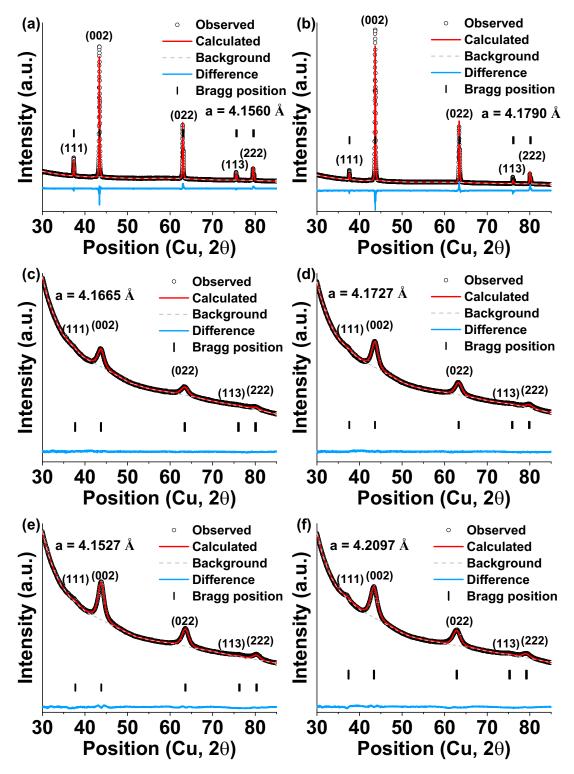
Increasing capacity in disordered rocksalt cathodes by Mg doping

Peichen Zhong^{1,2}, Zijian Cai^{1,2}, Yaqian Zhang^{1,2}, Raynald Giovine³, Bin Ouyang^{1,2}, Guobo Zeng^{1,2}, Yu Chen^{1,2}, Raphaële Clément³, Zhengyan Lun^{1,2}, and Gerbrand Ceder^{1,2}

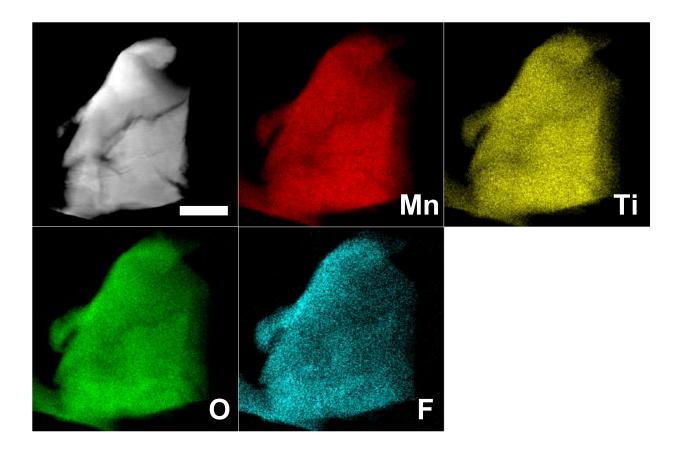
¹Department of Materials Science and Engineering, University of California Berkeley, Berkeley, California 94720, United States

²Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

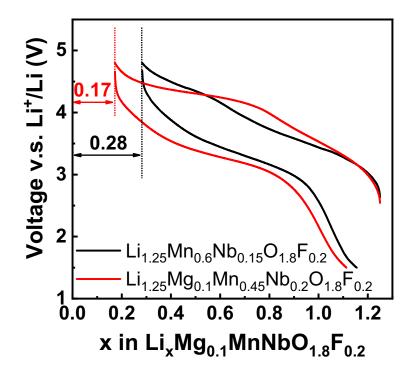
³Materials Department, University of California Santa Barbara, Santa Barbara, California 93106, United States



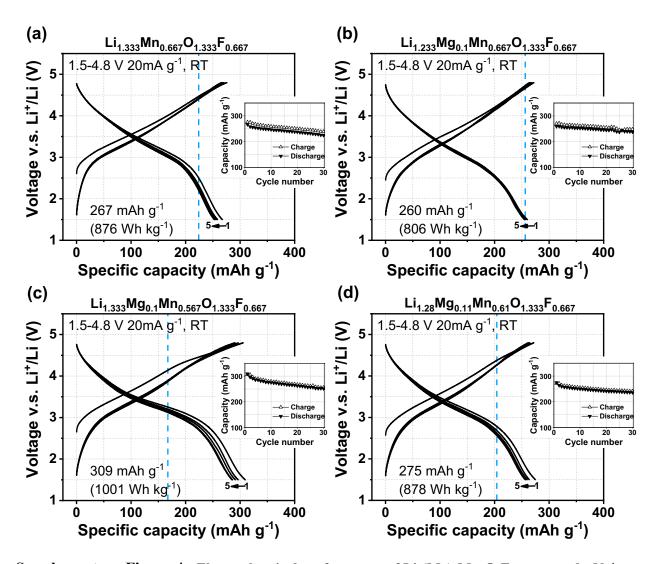
Supplementary Figure 1. XRD refinement of (a) LMTF, (b) LMMNF, (c) LMF, (d) LMMF, (e) ls-LMF, and (f) ms-LMF.



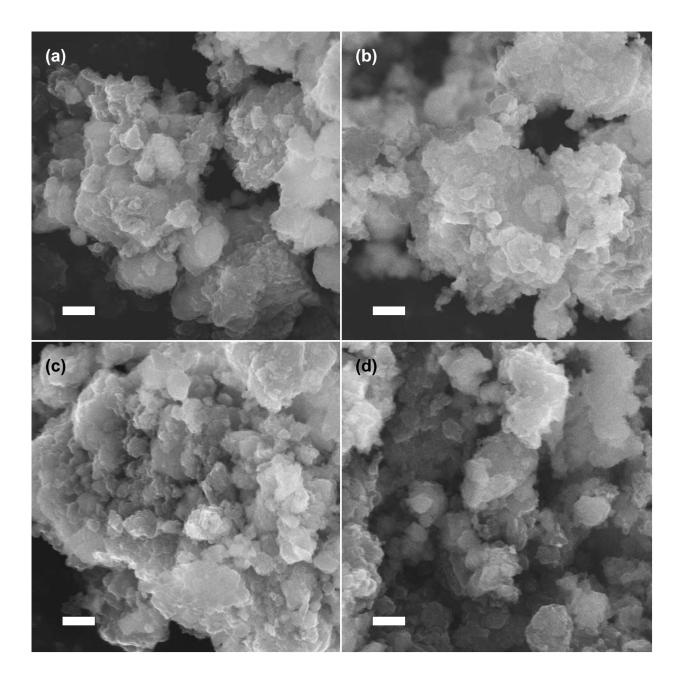
Supplementary Figure 2. TEM-EDS mapping of the element distribution in a representive particle of as-synthesized LMTF (scale bar, 300 nm)



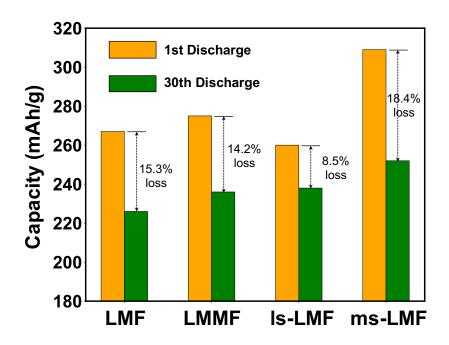
Supplementary Figure 3. Electrochemical performance of Li-(Mg)-Mn-Nb-O-F compounds. First cycle voltage profiles of Li_{1.25}Mn_{0.6}Nb_{0.15}O_{1.8}F_{0.2} (black) and Li_{1.25}Mg_{0.1}Mn_{0.45}Nb_{0.2}O_{1.8}F_{0.2} (red) within voltage window of 1.5 - 4.8V at 20 mA g⁻¹ at room temperature. The amount of remaining Li per f.u. at top of charge is shown in the figure.



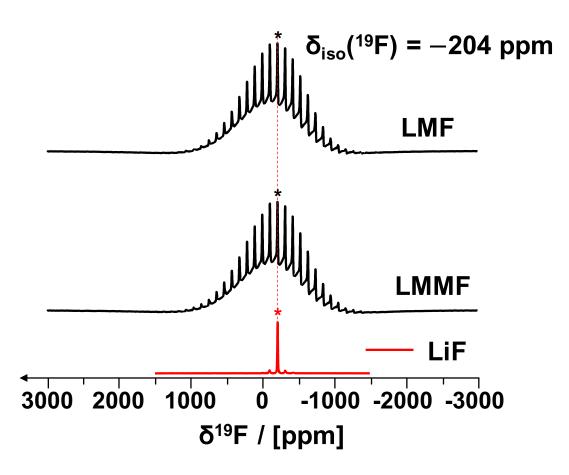
Supplementary Figure 4. Electrochemical performance of Li-(Mg)-Mn-O-F compounds. Voltage profile of the first 5 cycles and capacity retention of (a)LMF, (b) ls-LMF, (c) ms-LMF and (d) LMMF within voltage window of 1.5 - 4.8V at 20 mA g⁻¹ at room temperature. The blue dash lines indicate the theoretical Mn-redox capacity.



Supplementary Figure 5. Scanning electron microscope (SEM) images of (**a**) LMF, (**b**) LMMF, (**c**) ls-LMF and (**d**) ms-LMF that show the agglomeration of primary particles into secondary particles (scale bars, 400 nm).



Supplementary Figure 6. Cyclability comparison of LMF-based samples. The first discharge (orange) and the 30th discharge (green) capacity of LMF, LMMF, ls-LMF and ms-LMF samples are shown. The percentage of capacity loss is labeled in figure.



Supplementary Figure 7. ¹⁹F spin echo MAS NMR spectra of LMF and LMMF. For comparison, ¹⁹F spin echo spectra collected under similar experimental conditions ($B_0 = 7.05$ T) on a LiF powder sample are shown in red. The isotropic shift of the sharp resonance corresponding to ¹⁹F nuclei in LiF-like environments in the ¹⁹F NMR spectra is denoted with an asterisk. Spinning sidebands due to fast rotation of the samples during data acquisition are observed on either side of the isotropic signals.