Understanding Cation-Disordered Rocksalt Oxyfluoride Cathodes

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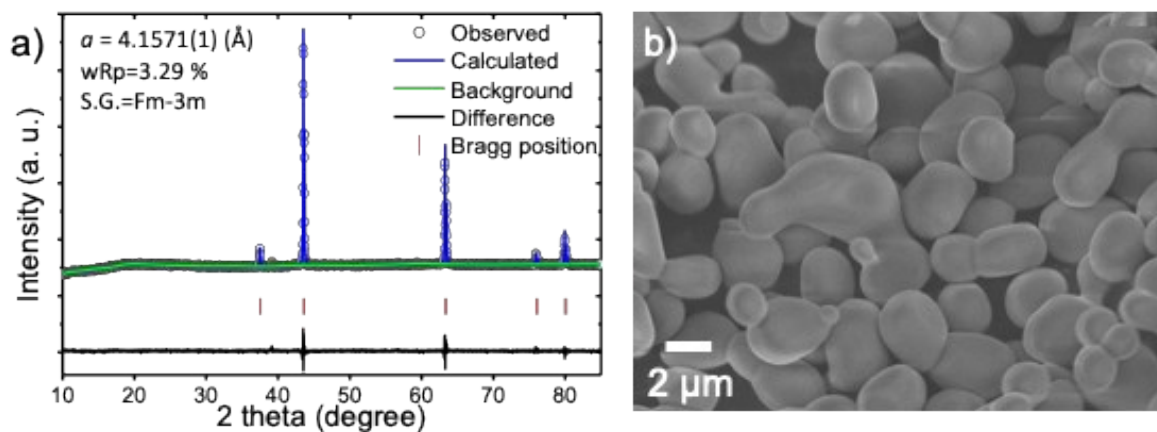
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Figure S1. a) XRD pattern and b) SEM image collected on pristine LTMO3.0.
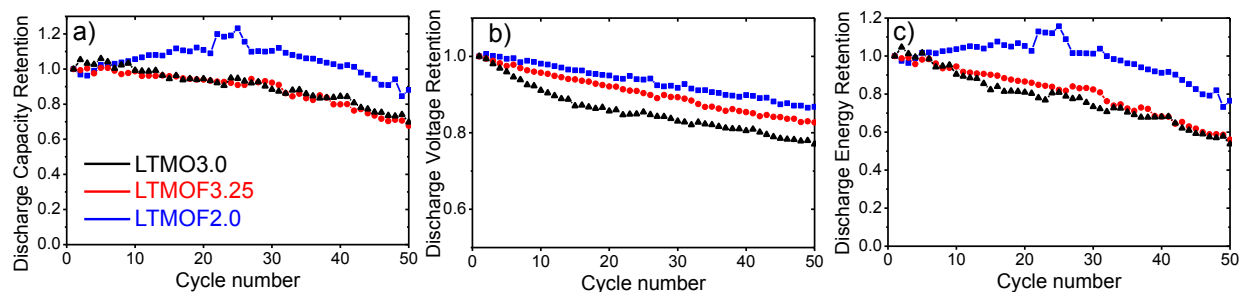

Figure S2. Comparison of discharge retention in: a) capacity, b) voltage and c) energy of LTMO3.0, LTMOF3.25 and LTMOF2.0 cathodes. The current density was 10 mA/g.
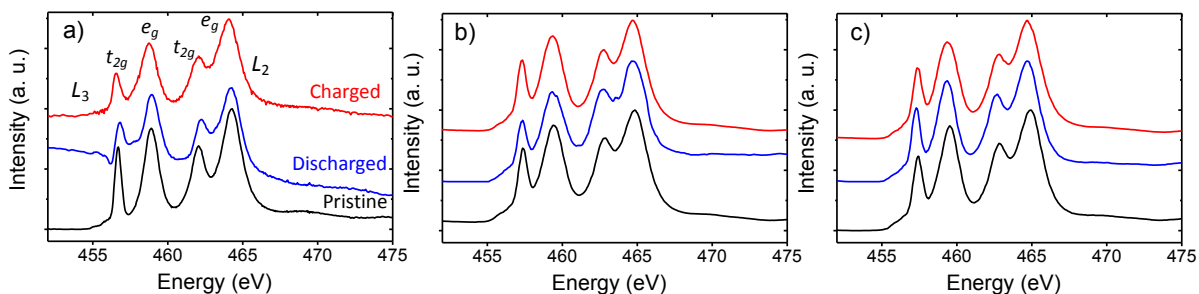
Figure S3. Ti *L*-edge XAS profiles collected on pristine, 1st charged (4.8 V) and 1st discharged (1.5 V) electrodes: a) LTMO3.0, b) LTMOF3.25 and c) LTMOF2.0
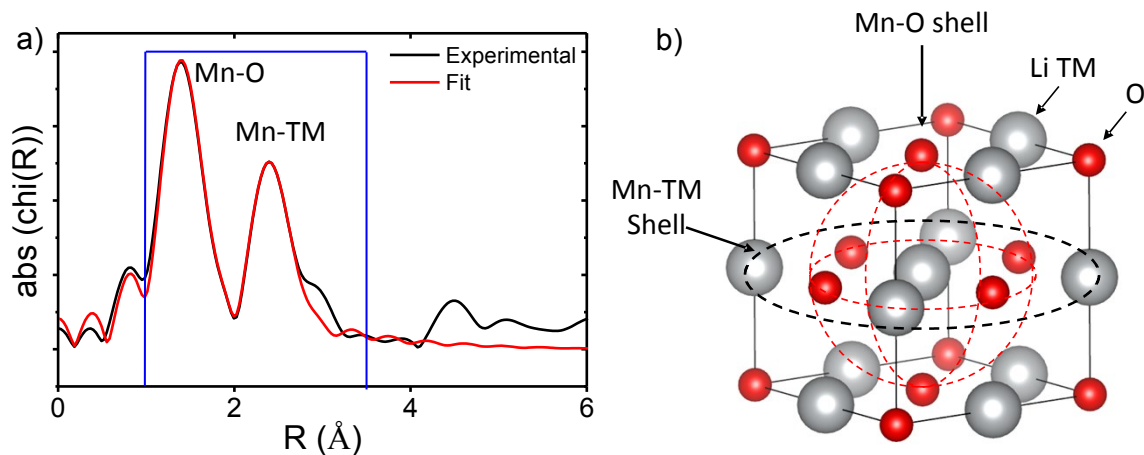

Figure S4. a) EXAFS profile and profile fitting of LTMOF3.25 using the first and second shells only and b) rocksalt structural model used for the fitting. The blue window in a) indicates the R range for the fitting.
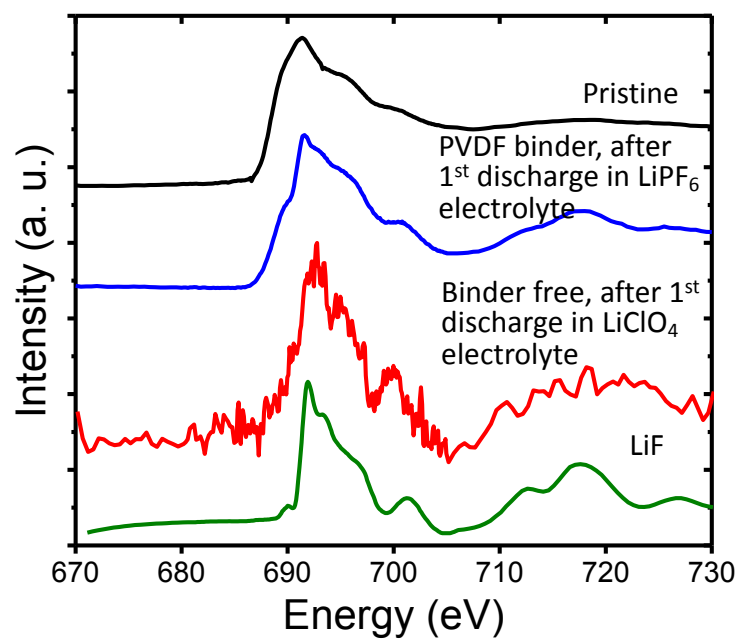
Figure S5. Comparison of F *K*-edge XAS profiles collected on LiF reference and LTMOF2.0 cathodes as indicated.

Table S1. Structural parameters of pristine LTMO3.0, LTMOF3.25 and LTMOF2.0 crystal samples determined from Rietveld refinement of X-ray diffraction patterns. Chemical compositions were determined by combined ICP and F-ISE measurements.

$Li_{1.2}Ti_{0.4}Mn_{0.4}O_2$ (LTMO3.0), Li: Ti: Mn = 1.197: 0.393: 0.410, $Fm\overline{3}m$, a (Å) = 4.1571

Atom	Position	Wyck. Site	Occupancy	d(M-O) (Å)
Li	0, 0, 0	$4a$	0.56	2.0784
Ti	0, 0, 0	$4a$	0.22	2.0784
Mn	0, 0, 0	$4a$	0.22	2.0784
O	0, 0, 0.5	$4b$	1.0	-

$Li_{1.3}Ti_{0.3}Mn_{0.4}O_{1.7}F_{0.3}$ (LTMOF3.25), Li: Ti :Mn :F = 1.316: 0.282: 0.401: 0.33, $Fm\overline{3}m$, a (Å) = 4.1577

Atom	Position	Wyck. site	Occupancy	d(M-O) (Å)
Li	0, 0, 0	$4a$	0.65	2.0781
Ti	0, 0, 0	$4a$	0.12	2.0781
Mn	0, 0, 0	$4a$	0.23	2.0781
O	0, 0, 0.5	$4b$	0.82	-
F	0, 0, 0.5	$4b$	0.18	-

$Li_{1.2}Ti_{0.2}Mn_{0.6}O_{1.8}F_{0.2}$ (LTMOF2.0), Li: Ti: Mn: F = 1.191: 0.201: 0.605: 0.19, $Fm\overline{3}m$, a (Å) = 4.1572

Atom	Position	Wyck. Site	Occupancy	d(M-O) (Å)
Li	0, 0, 0	$4a$	0.60	2.0781
Ti	0, 0, 0	$4a$	0.10	2.0781
Mn	0, 0, 0	$4a$	0.30	2.0781
O	0, 0, 0.5	$4b$	0.92	-
F	0, 0, 0.5	$4b$	0.08	-