

Supporting Information

Phase Separation and d Electronic Orbitals on Cyclic Degradation in Li-Mn-O Compounds: First-Principles Multiscale Modeling and Experimental Observations

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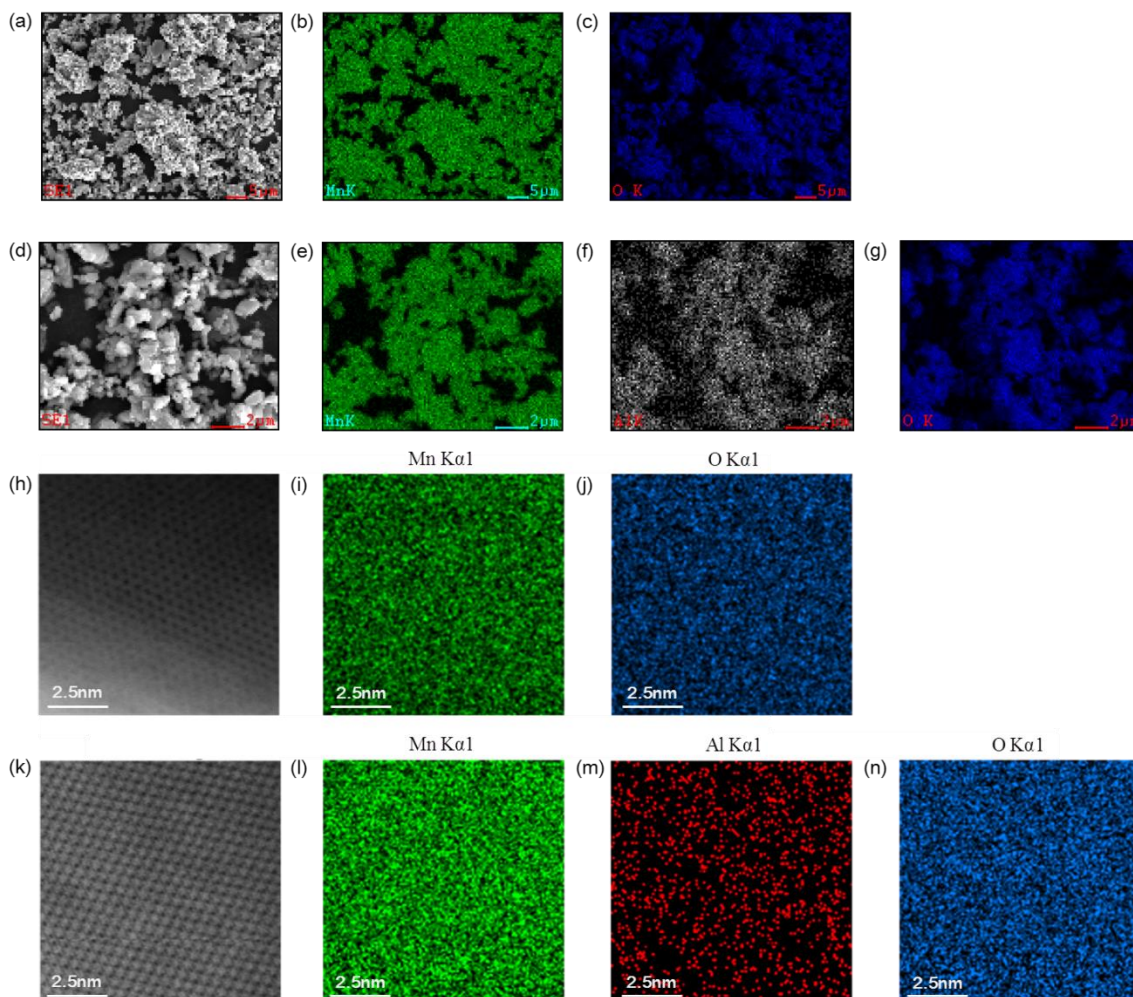


Figure S1. FESEM images of (a) LMO and (d) LMAO, corresponding EDS elemental mapping of (b and e) Mn (green), (f) Al (gray), and (c and g) O (blue). STEM images of (h) LMO and (k) LMAO with EDS elemental mapping of (i and l) Mn (green), (m) Al (red), and (j and n) O (blue).

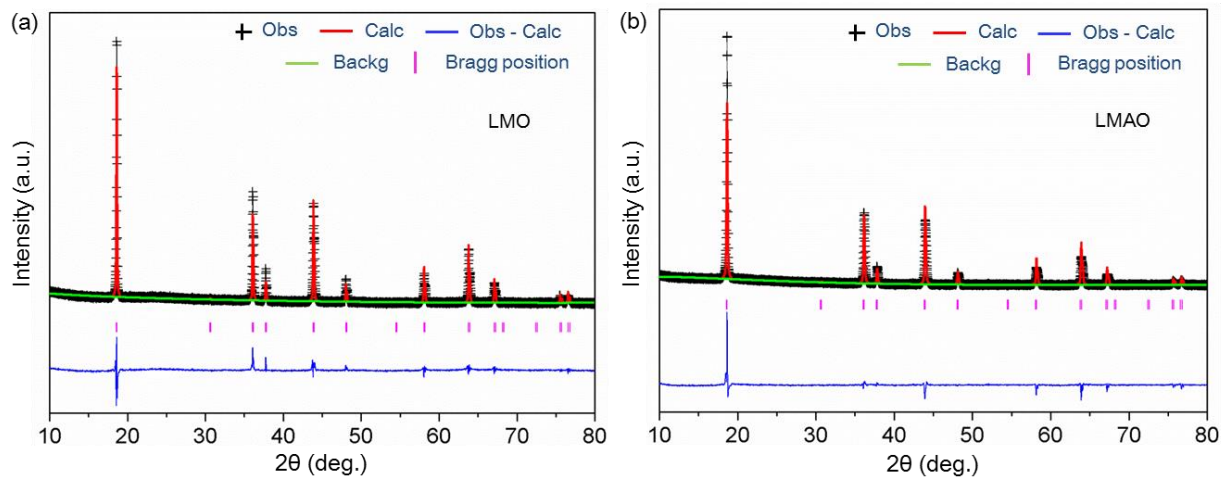


Figure S2. Rietveld refinement data from X-ray diffraction patterns of (a) LMO and (b) LMAO.

Compounds	Region	\mathcal{E}_i^f [eV]	\mathcal{K}_i^f [eV·nm ²]
LMO	0.0 ~ 0.125	0.0	0.0
	0.125 ~ 0.375	44.7386	5.7696
	0.375 ~ 1.0	4.0689	0.5247
LMAO	0.0 ~ 0.25	0.0	0.0
	0.25 ~ 0.625	14.2982	1.8538
	0.625 ~ 0.875	31.0502	4.0257
	0.875 ~ 1.0	0.0	0.0

Table S1. First-principles bulk free energy coefficient, \mathcal{E}_i^f , and the corresponding gradient energy coefficient, \mathcal{K}_i^f , at various reaction regions in LMO and LMAO.