Supporting Information

Site Dependent Multicomponent Doping Strategy for Ni–rich $LiNi_{1-2y}Co_yMn_yO_2$ (y = 1/12) Cathode Materials for Li–Ion Batteries

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Table S1. The calculated total energy used in calculating heat of formation. The total energy of Li and O are -1.898 and -4.225 eV/atom. Noted the total energy of O is obtained after adding a correction term for the O2 molecule, which compensate the DFT over–delocalization of oxygen p orbitals, and improve the accuracy of the obtained heats of formation.

Dopant	Total Energy (eV/24 formula unit $LiMO_2$)				Dopant oxides	Cell Size (formula unit M_xO_y)	Total Energy (eV/cell)
	Co site	Li site	Mn site	Ni site			
Al	-479.301	-481.025	-474.345	-481.743	Al2O3	6	-226.48
Ga	-475.518	-477.443	-470.559	-478.121	Ga2O3	4	-121.387
Mg	-474.422	-476.522	-469.363	-476.823	MgO	4	-48.4143
Si	-481.878	-483.404	-476.882	-484.391	SiO2	4	-95.6421
Ti	-484.778	-487.048	-479.765	-487.417	TiO2	8	-213.107
V	-482.223	-484.512	-477.356	-484.922	V2O5	4	-104.834
Zr	-484.425	-486.796	-479.413	-487.024	ZrO2	4	-108.521

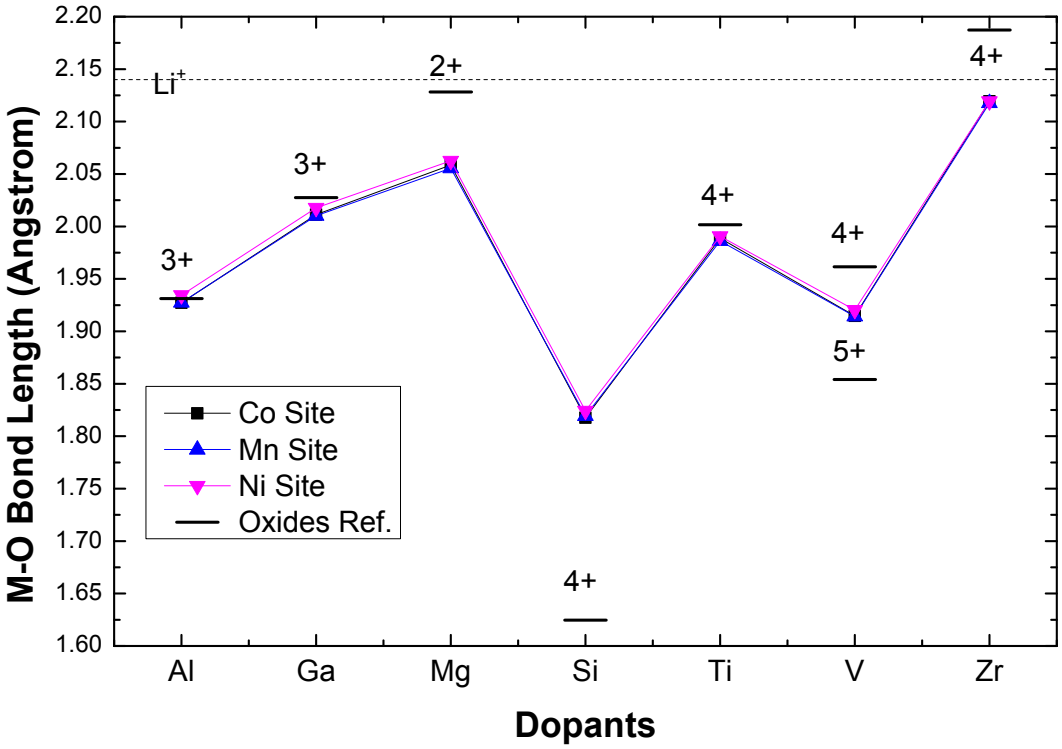

Figure S1. Dopant-O bond length for the seven dopants considered: Al, Ga, Mg, Si, Ti, V and Zr. The reference bond lengths are derived from the most stable binary oxides: Al_2O_3, Ga_2O_3, MgO, SiO_2, TiO_2, V_2O_5, VO_2 and ZrO_2, respectively. The dotted line is the bond length of Li-O in Ni-rich NCM.

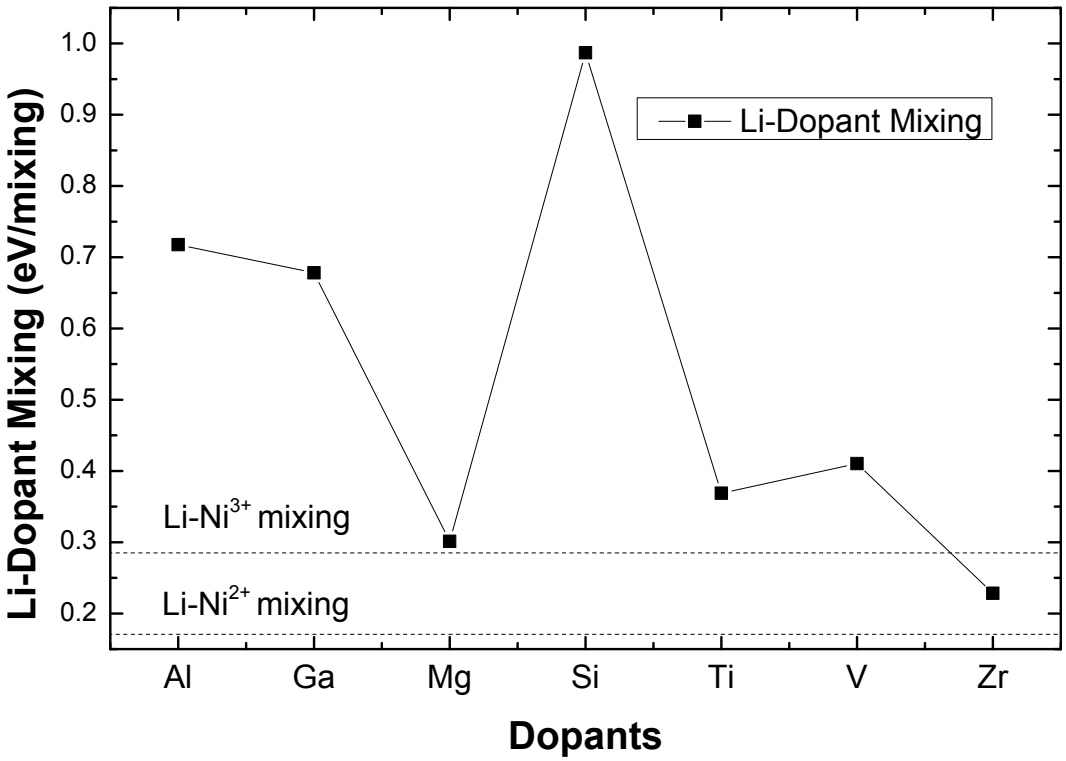

Figure S2. Formation energy of Li-dopant exchange. The energy of Li-Ni exchange in pristine Ni-rich NCM is also shown for comparison.

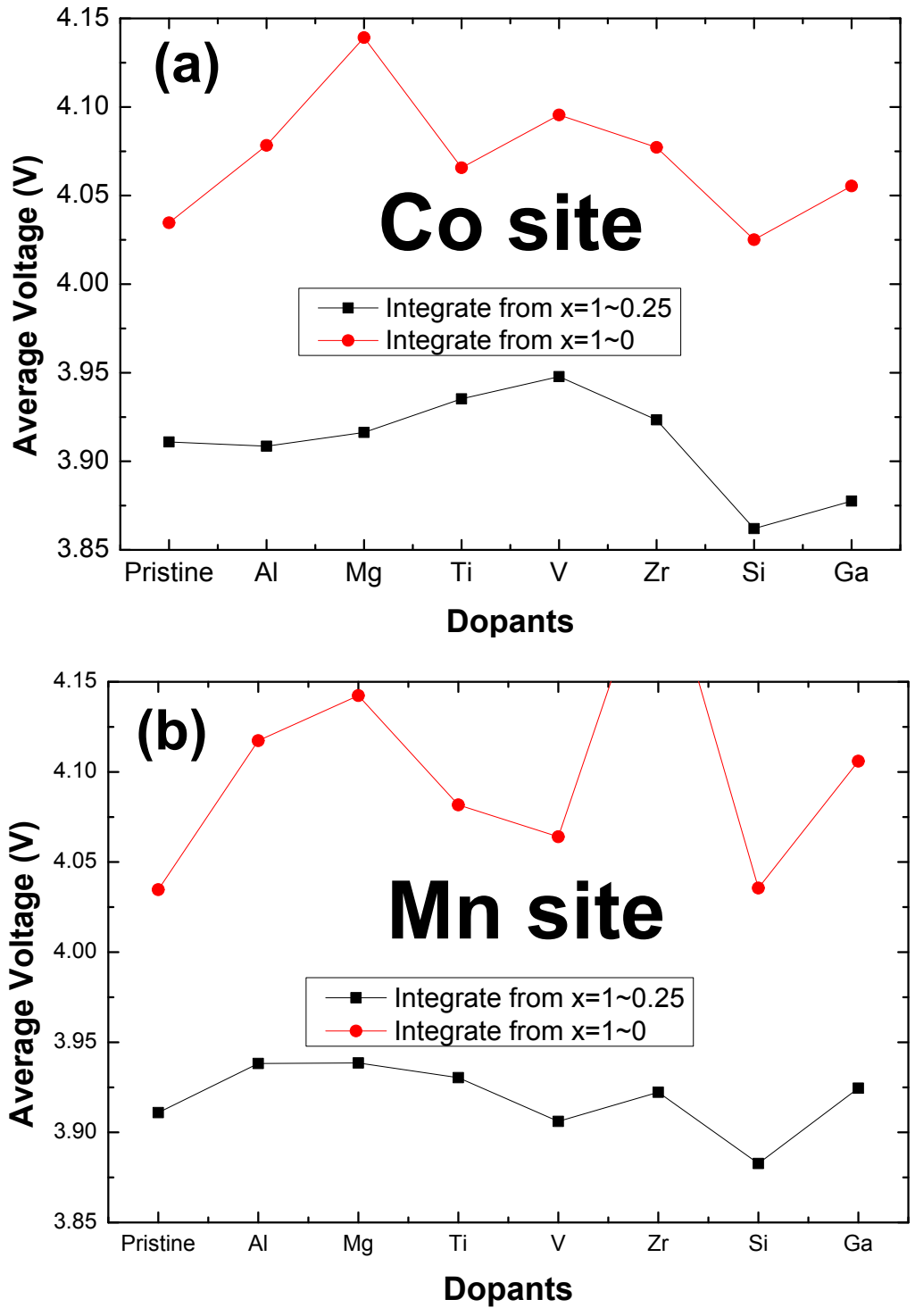

Figure S3. Calculated average voltage of NCM811 with or without dopants, (a) at Co sites, (b) at Mn sites.