Supporting Information

Role of Fluorine Surface Modification in Improving Electrochemical Cyclability of Concentration Gradient Li[Ni0.73Co0.12Mn0.15]O2 Cathode Material for Li-Ion Batteries

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Table S1. Atom parameters of the pristine CG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_2$ and FMCG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{1.99}F_{0.01}$ materials (space group = R-m, occ = site occupancy)

$Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_2$			Rwp: 5.8%	Rp: 2.9%	$Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{1.99}F_{0.01}$			Rwp: 5.0%	Rp: 2.7%
	x	y	z	occ		x	y	z	occ
Li (3a)	0	0	0	0.9851	Li (3a)	0	0	0	0.9846
Li (3b)	0	0	0.5	0.0149	Li (3b)	0	0	0.5	0.0154
Ni (3a)	0	0	0	0.0149	Ni (3a)	0	0	0	0.0154
Ni (3b)	0	0	0.5	0.7151	Ni (3b)	0	0	0.5	0.7146
Co (3b)	0	0	0.5	0.12	Co (3b)	0	0	0.5	0.12
Mn (3b)	0	0	0.5	0.15	Mn (3b)	0	0	0.5	0.15
O (6c)	0	0	0.259	2.00	O (6c)	0	0	0.259	1.99
F (6c)	0	0	0.259	0	F (6c)	0	0	0.259	0.01

Table S2. Atom parameters of the FMCG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{1.98}F_{0.02}$ and FMCG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{1.97}F_{0.03}$ materials (space group = R-m, occ = site occupancy).

$Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{1.98}F_{0.02}$			Rwp: 4.9%	Rp: 2.6%	$Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{1.97}F_{0.03}$			Rwp: 4.9%	Rp: 2.7%
	x	y	z	occ		x	y	z	occ
Li (3a)	0	0	0	0.9826	Li (3a)	0	0	0	0.9807
Li (3b)	0	0	0.5	0.0174	Li (3b)	0	0	0.5	0.0193
Ni (3a)	0	0	0	0.0174	Ni (3a)	0	0	0	0.0193
Ni (3b)	0	0	0.5	0.7126	Ni (3b)	0	0	0.5	0.7107
Co (3b)	0	0	0.5	0.12	Co (3b)	0	0	0.5	0.12
Mn (3b)	0	0	0.5	0.15	Mn (3b)	0	0	0.5	0.15
O (6c)	0	0	0.259	1.98	O (6c)	0	0	0.259	1.97
F (6c)	0	0	0.259	0.02	F (6c)	0	0	0.259	0.03

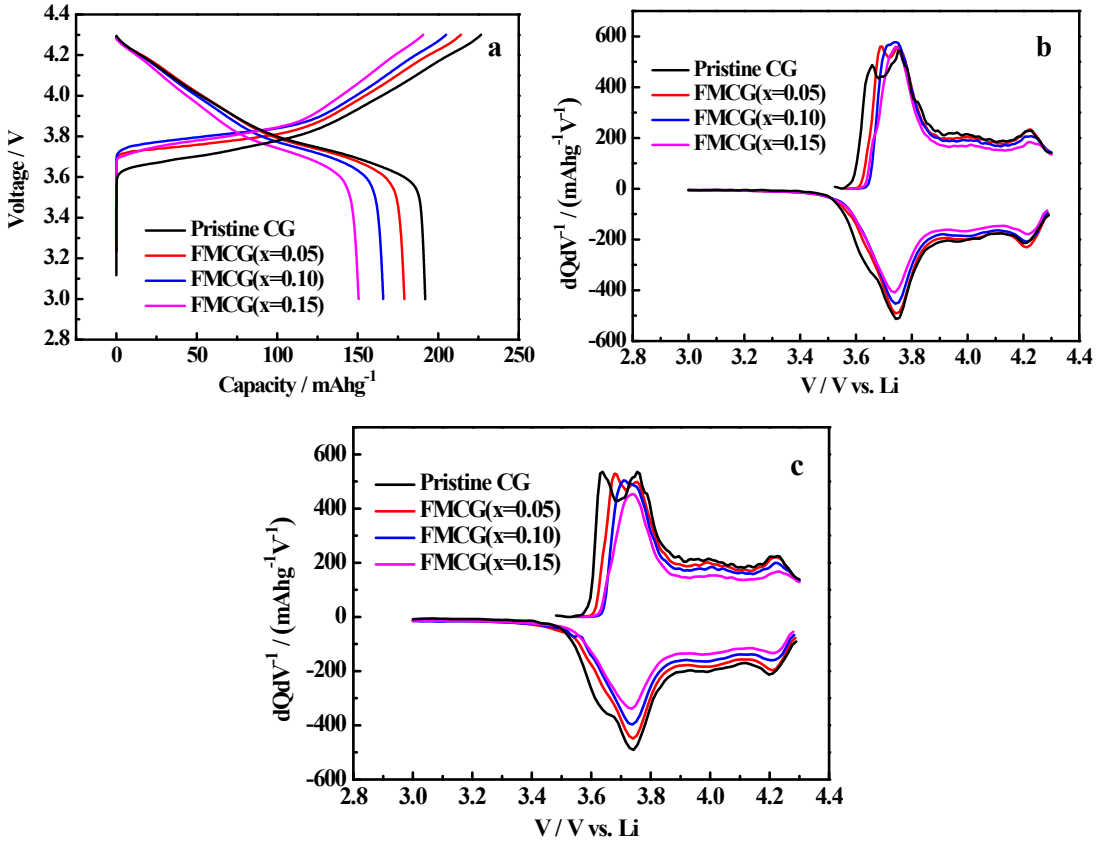

Figure S1. Initial capacities (a), and differential capacity profiles at the 2nd (b) and the 10th (c) cycles for the pristine CG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_2$ and FMCG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{2-x}F_x$ (x=0.05, 0.10 and 0.15) cathodes at the current rate of 0.1C between 4.3 V and 3.0 V.

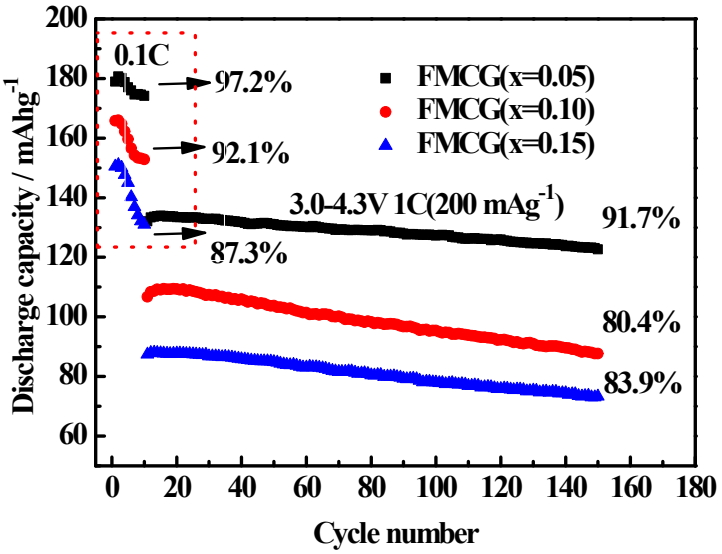

Figure S2. Cycling performance of the FMCG $Li[Ni_{0.73}Co_{0.12}Mn_{0.15}]O_{2-x}F_x$ (x=0.05, x=0.10 and x=0.15) cathodes at the current rate of 1C between 4.3 V and 3.0 V.