Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Developing O3 type layered oxide cathode and its application in 18650 commercial type Na-ion batteries

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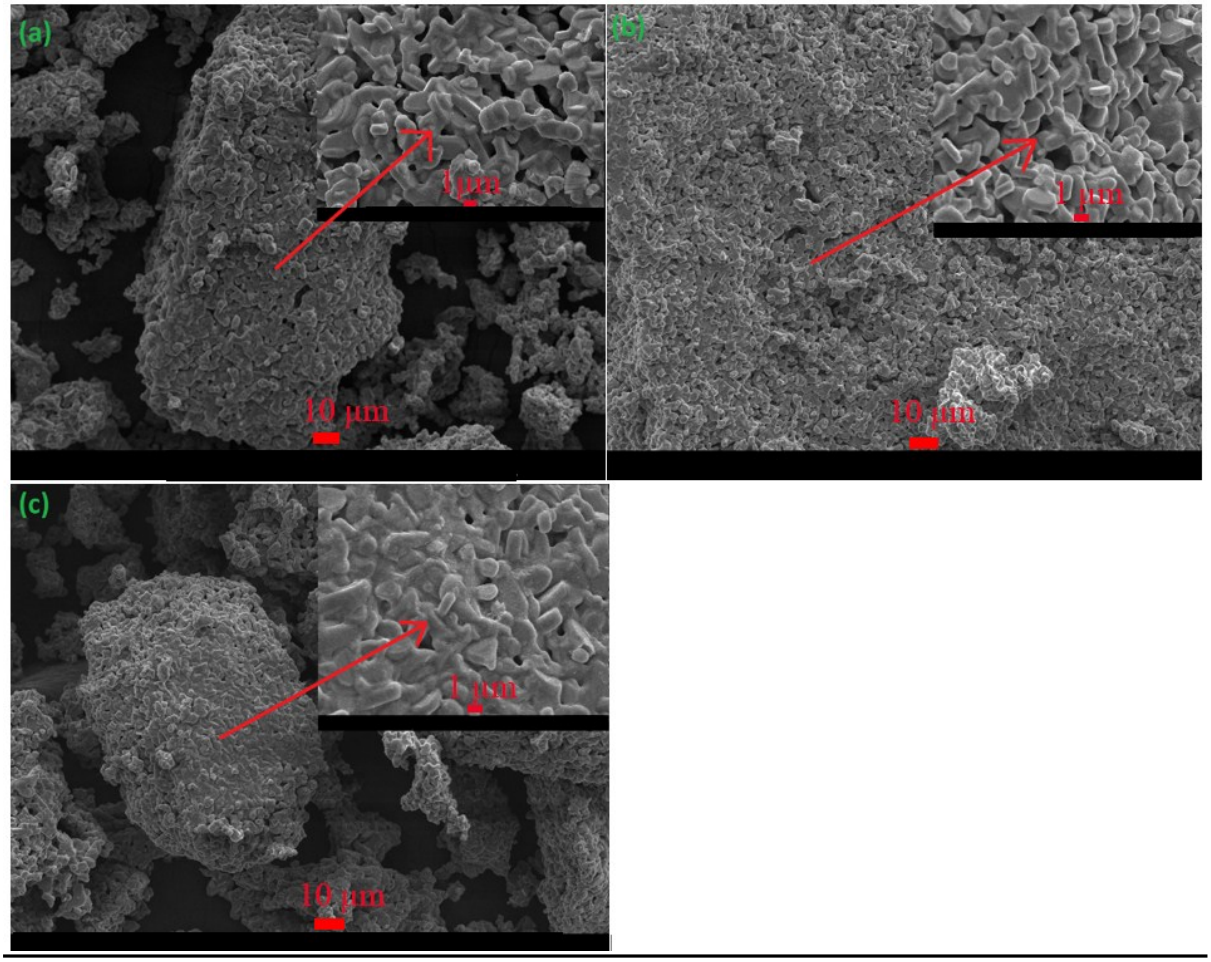

Figure S1: SEM images of (a) NCMF (b) NCMFT (c) NNCMFT at 550X and 4000X (inset).

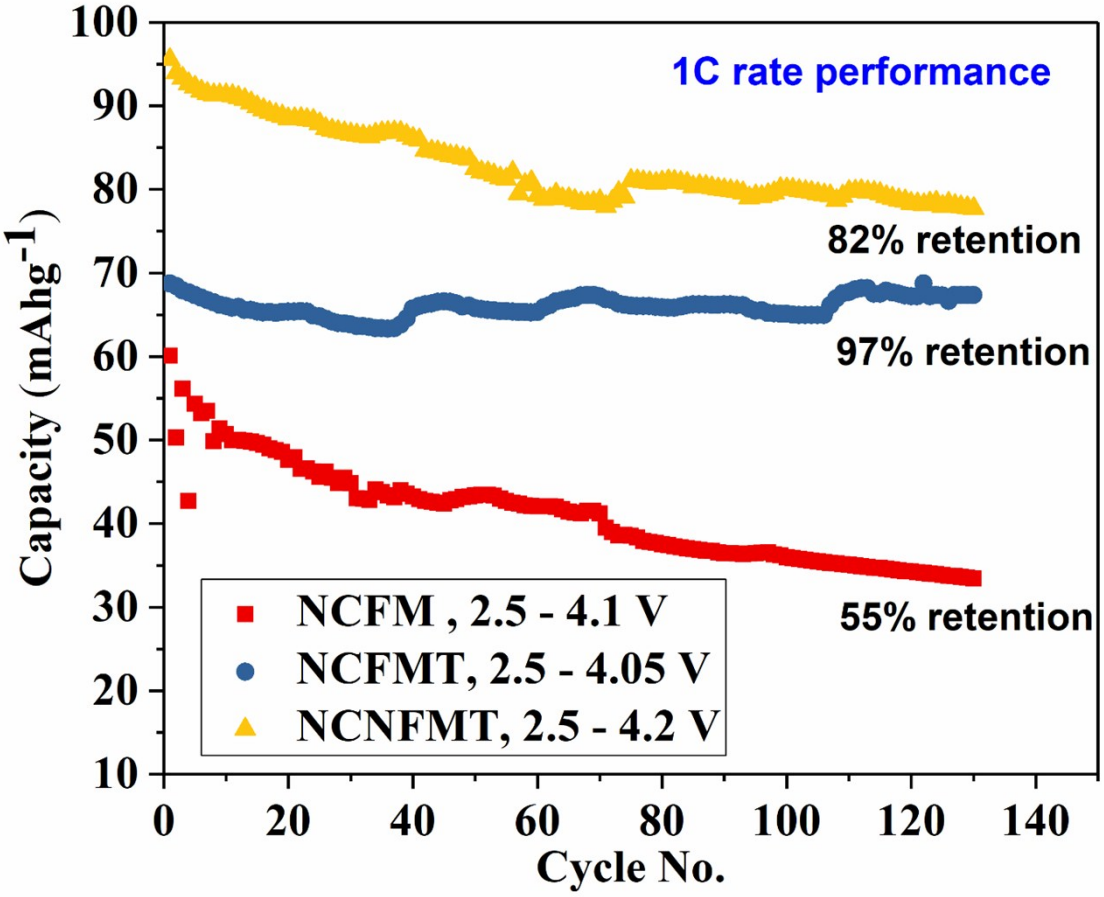

Figure S2: 1C cycling data for NCFM, NCFMT and NCNFMT.

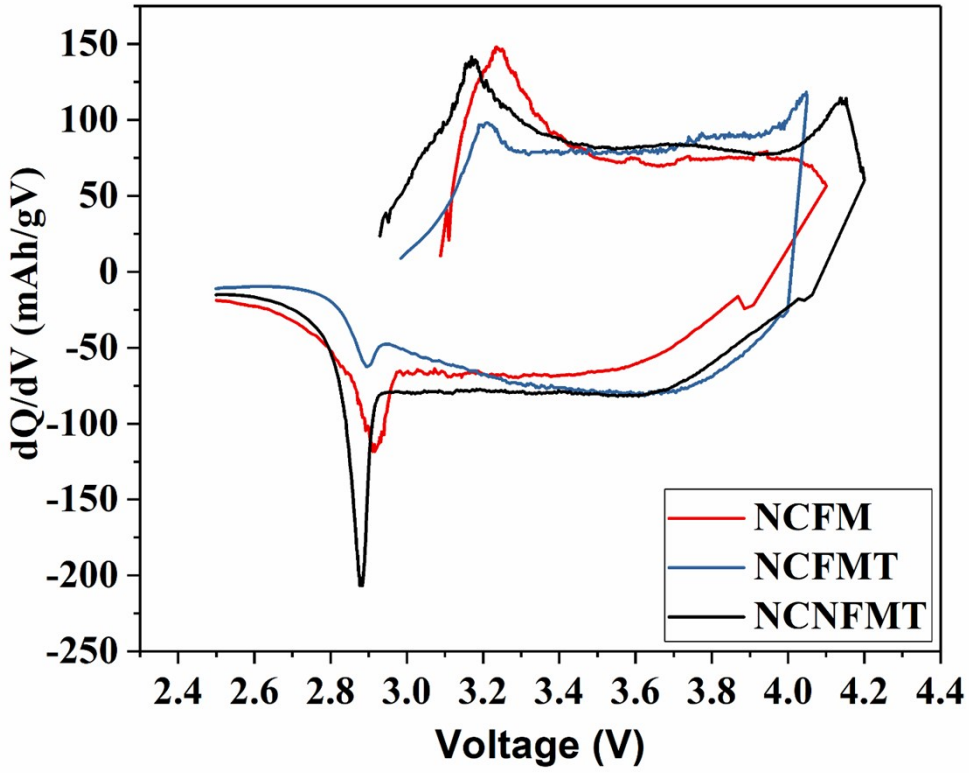

Figure S3: dQ/dV v/s Voltage plot of first cycle for NCFM, NCFMT and NCNFMT

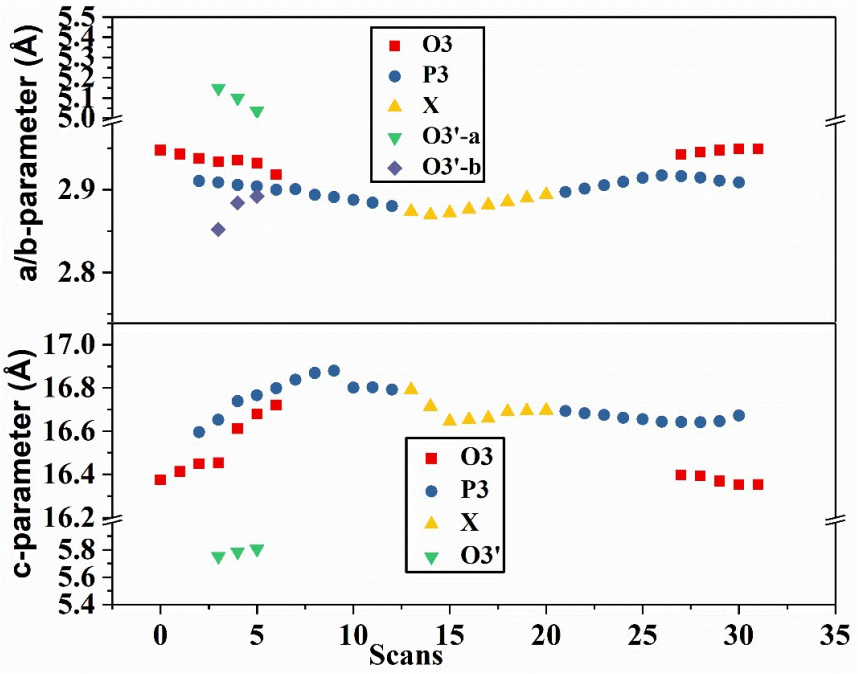

Figure S4: Lattice parameters of NCFM material during charge/discharge

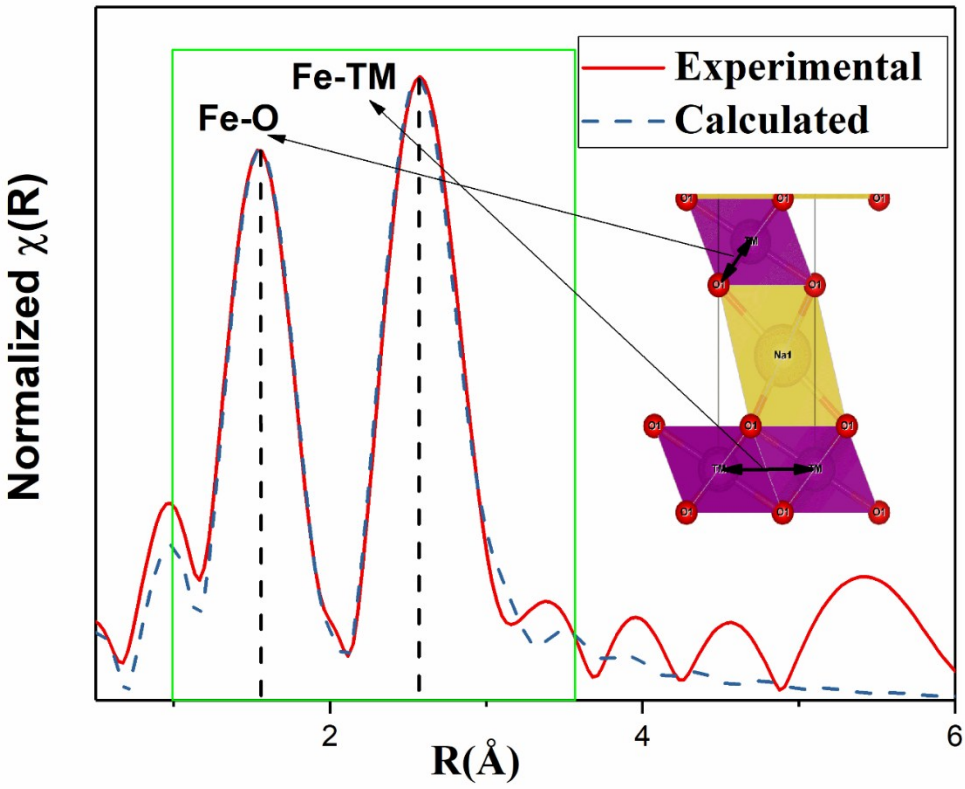

Figure S5: Fourier transform and the fit of first 2 coordination shells: Fe-O and Fe-TM.

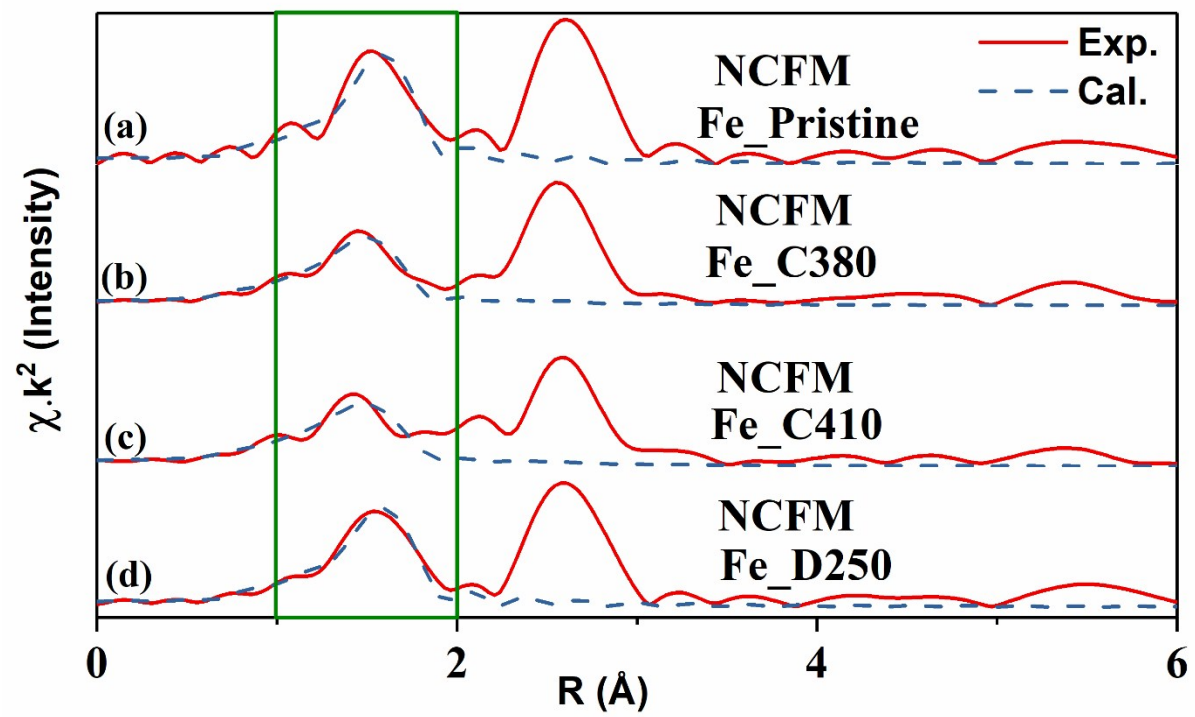

Figure S6: Fitting of EXAFS data for first shell of NCFM at Fe: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

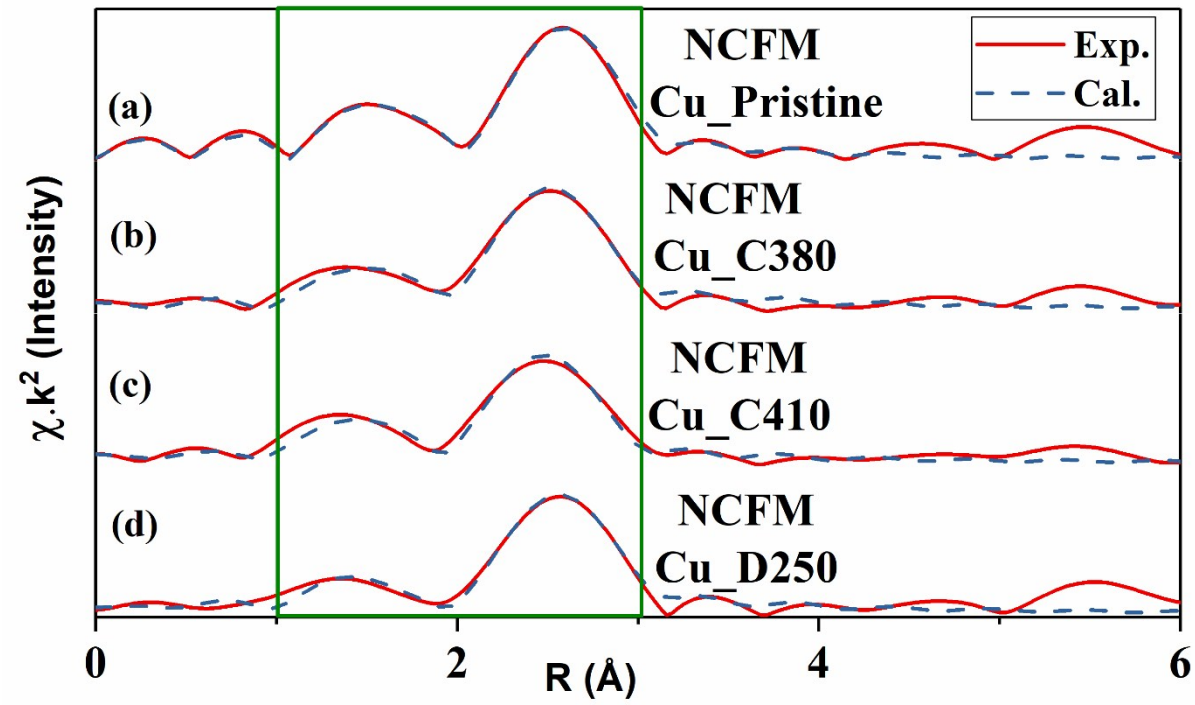

Figure S7: Fitting of EXAFS data for first shell for NCFM at Cu: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

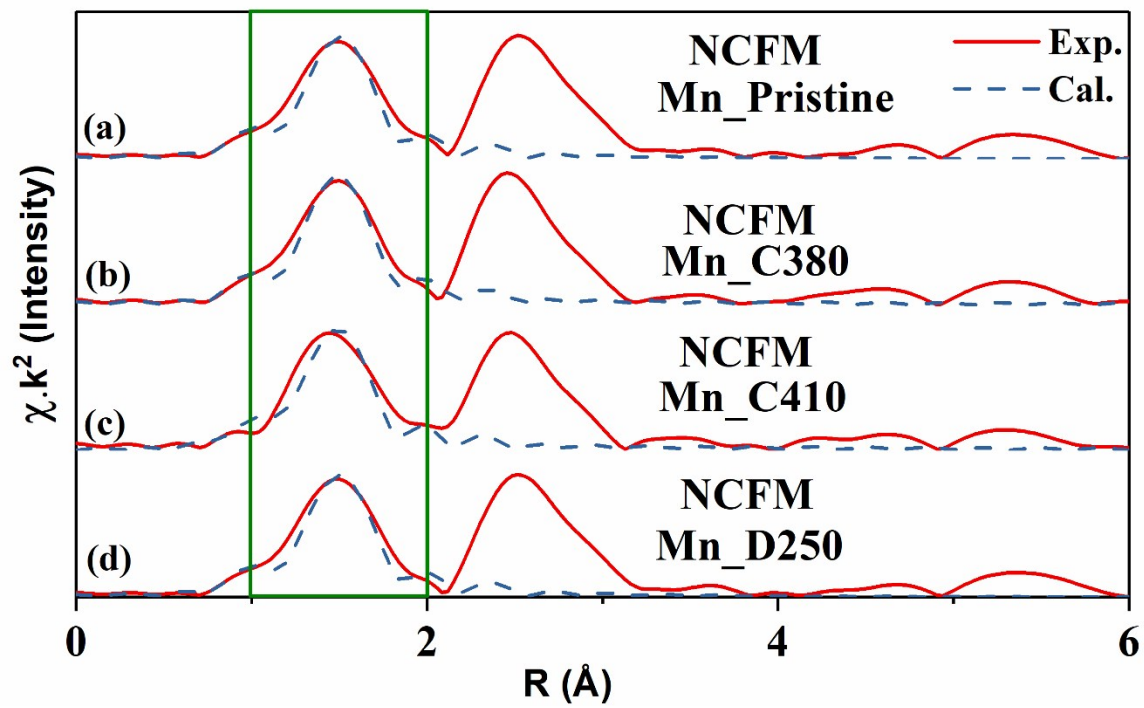

Figure S8: Fitting of EXAFS data for first shell for NCFM at Mn: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

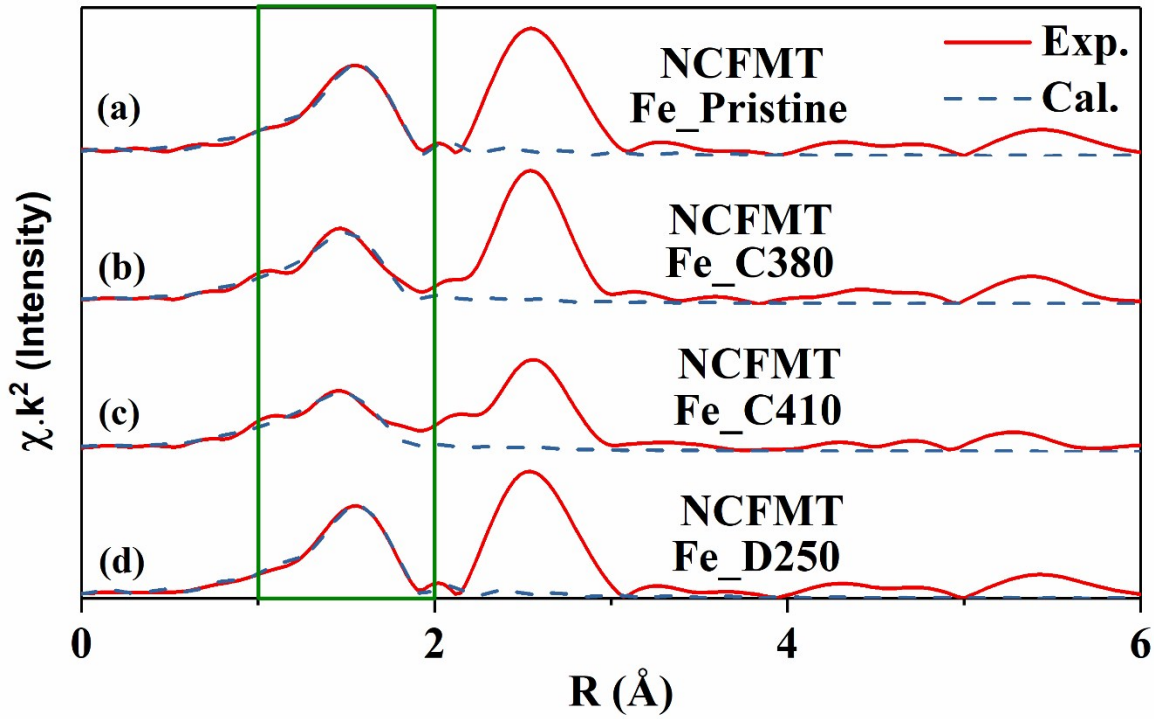

Figure S9: Fitting of EXAFS data for first shell for NCFMT at Mn: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

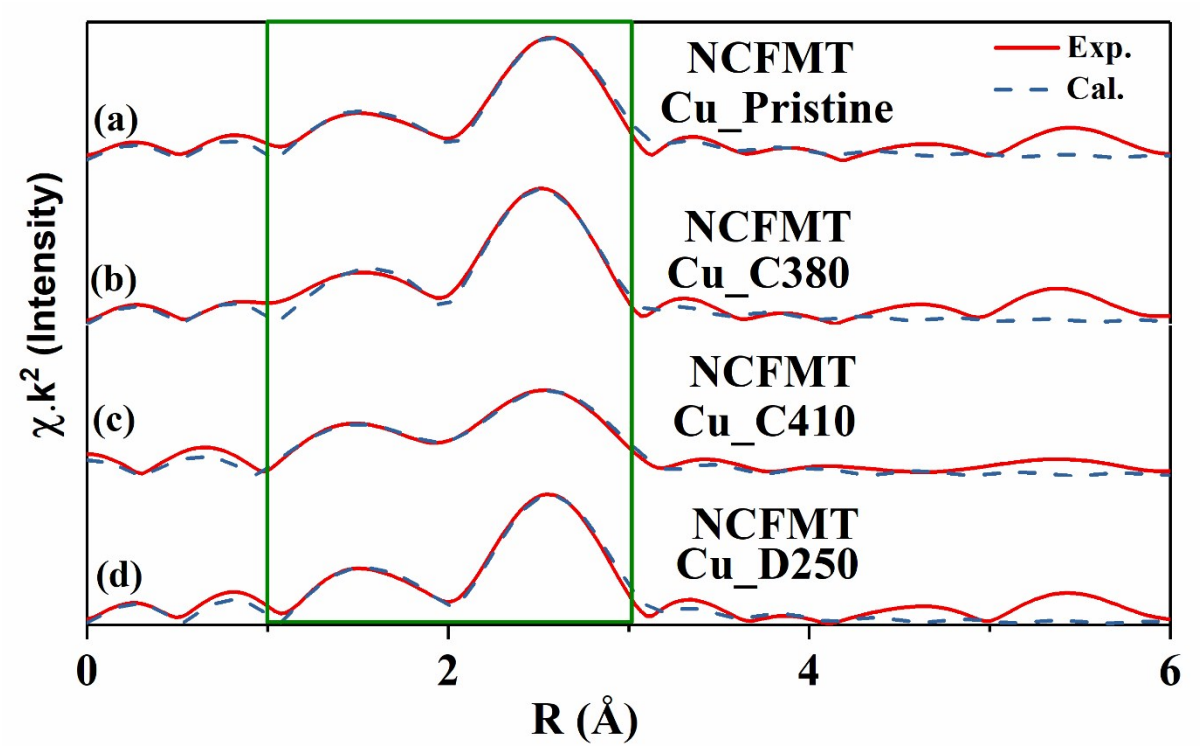

Figure S10: Fitting of EXAFS data for first shell for NCFMT at Cu: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

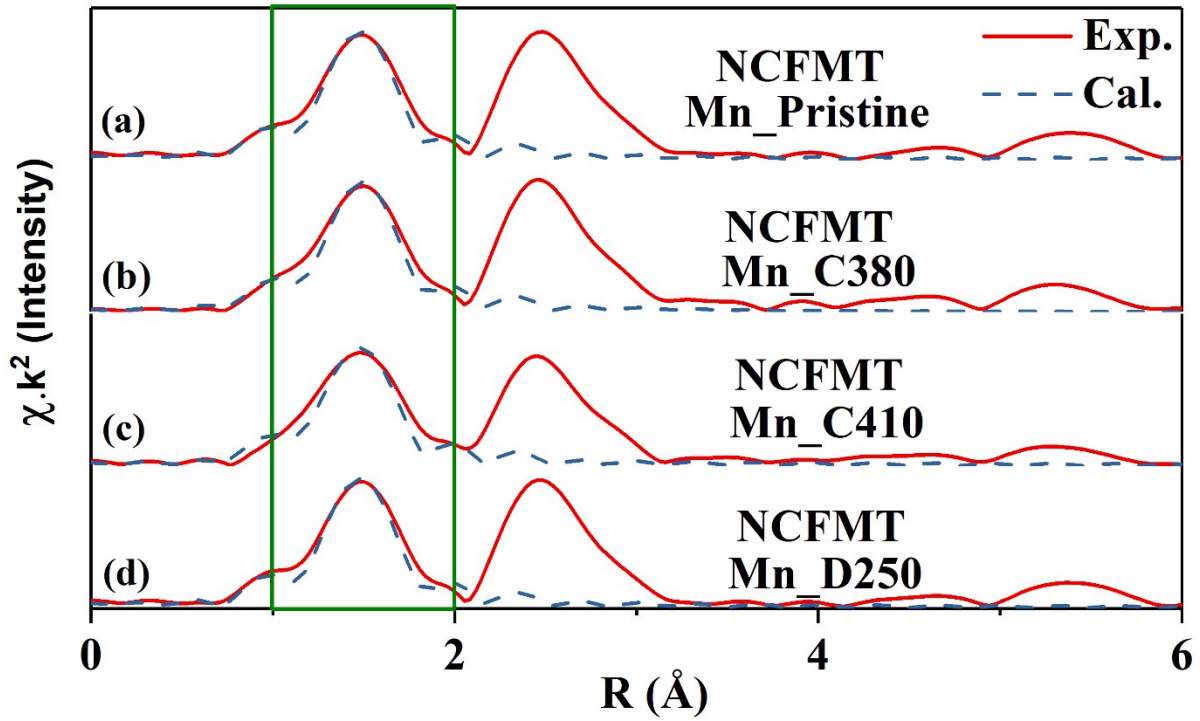

Figure S11: Fitting of EXAFS data for first shell for NCFMT at Mn: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

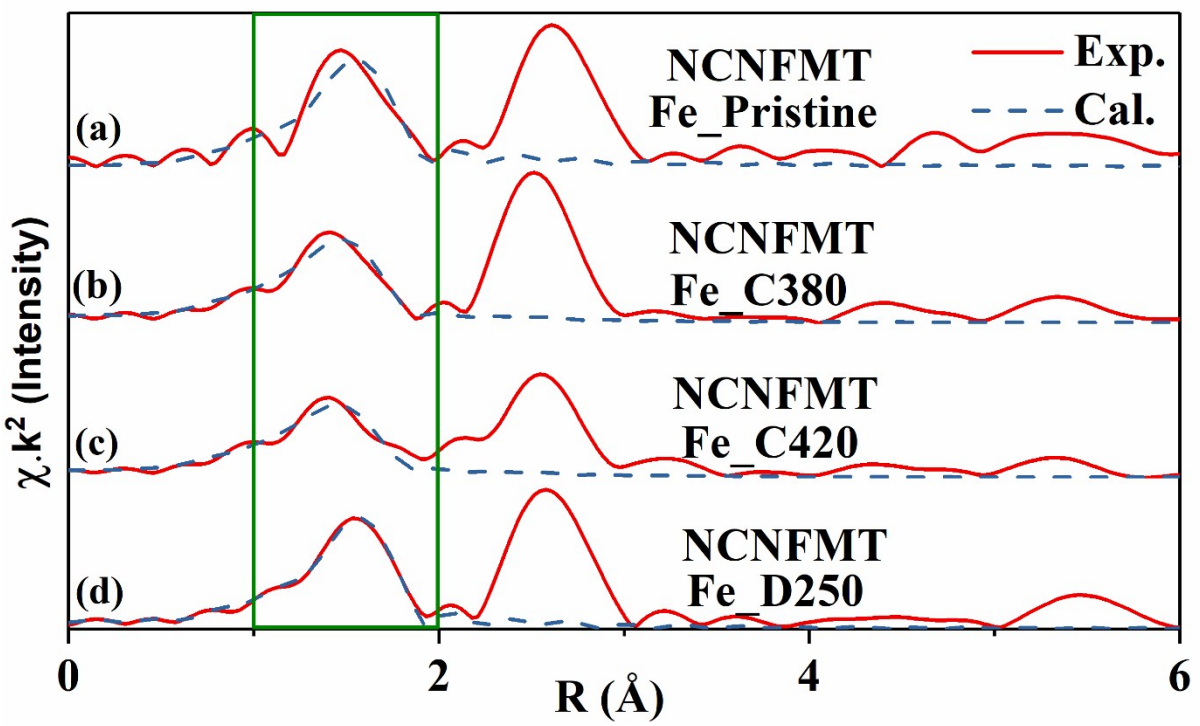

Figure S12: Fitting of EXAFS data for first shell for NCNFMT at Fe: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

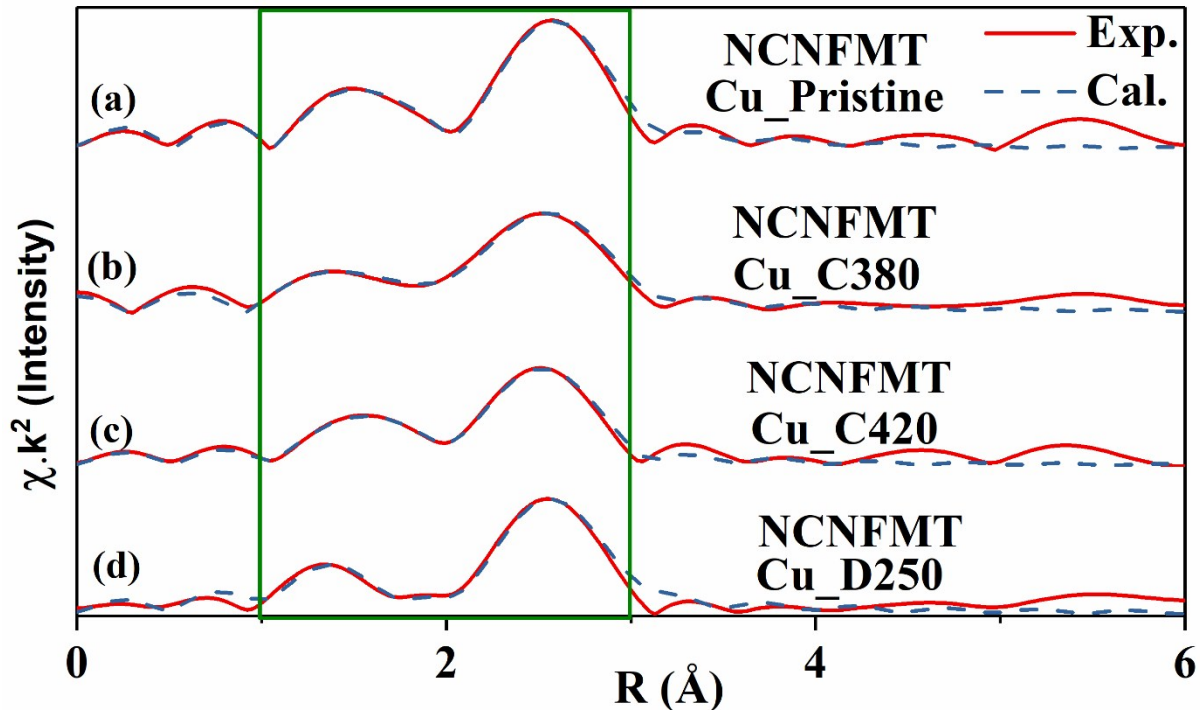

Figure S13: Fitting of EXAFS data for first shell for NCNFMT at Cu: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

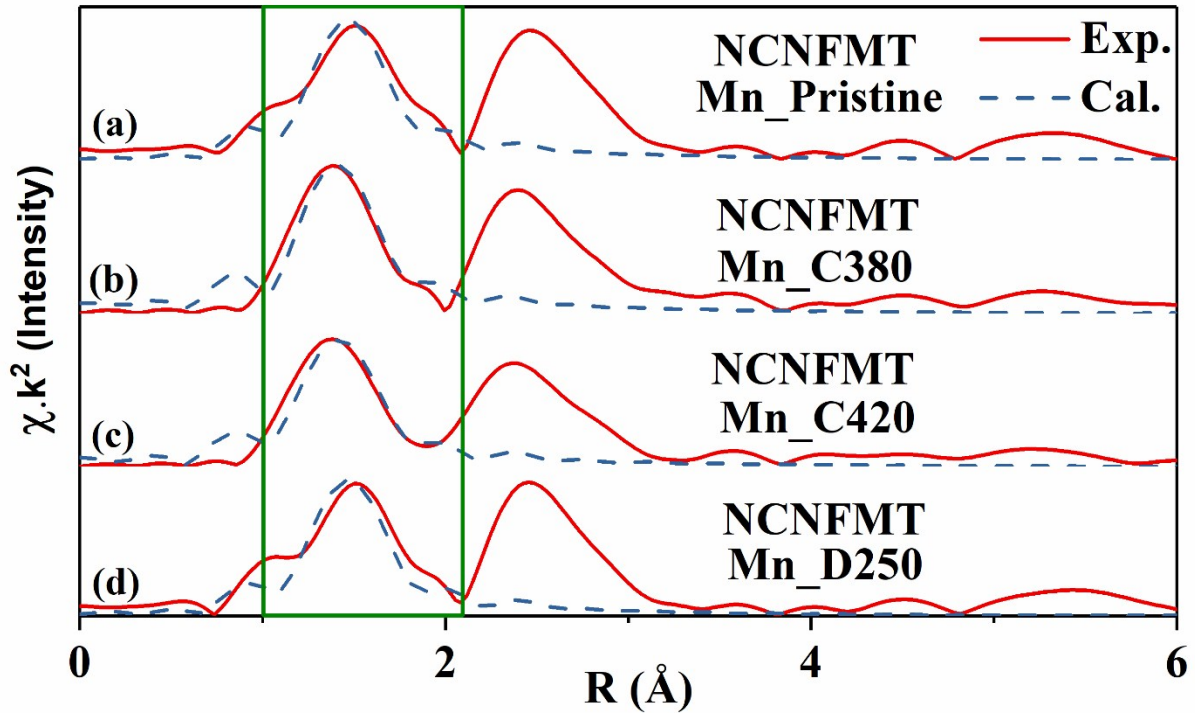

Figure S14: Fitting of EXAFS data for first shell for NCNFMT at Mn: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R

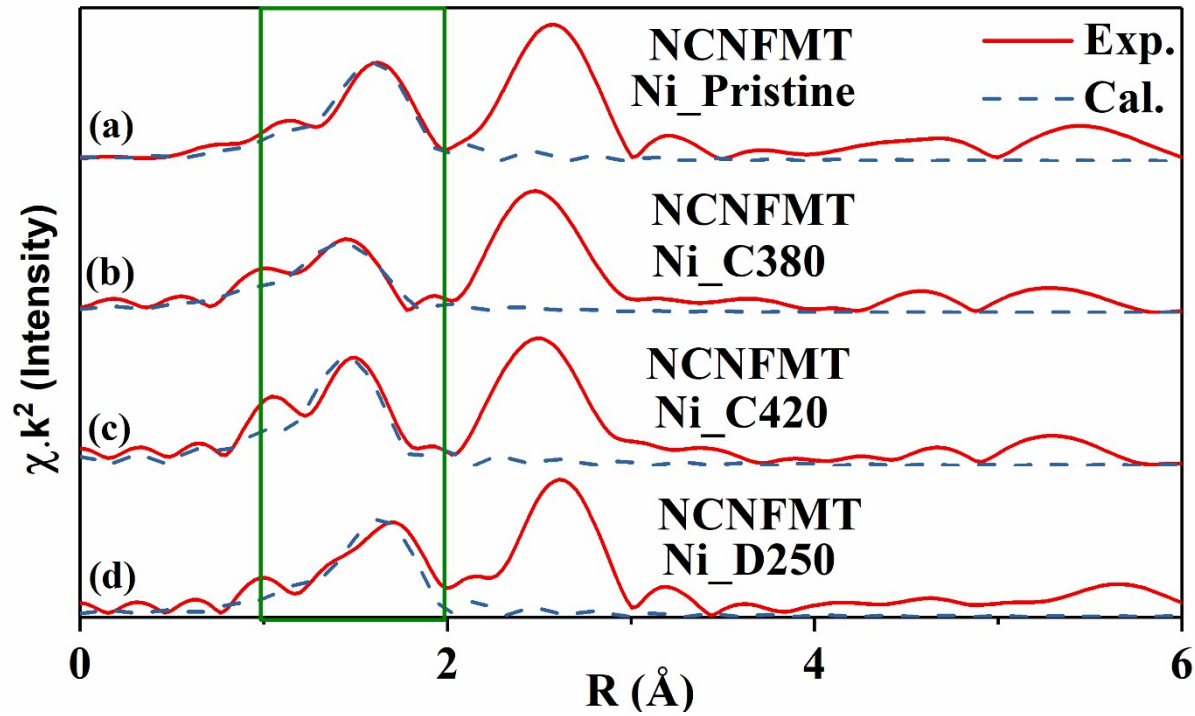

Figure S15: Fitting of EXAFS data for first shell for NCNFMT at Ni: (a) Pristine sample, (b) Sample desodiated till 3.8 V, (c) Sample desodiated till 4.1 V and (d) Sample sodiated till 2.5 V. Green box indicates the range of fit in R.

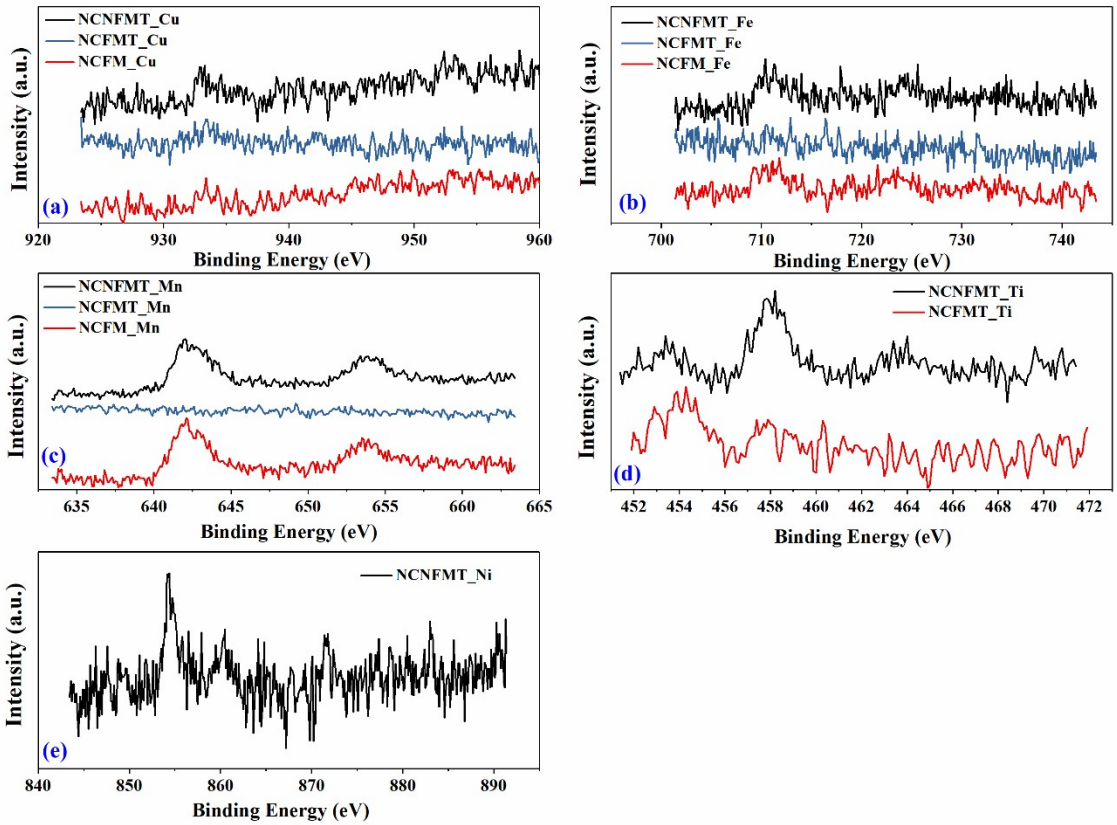

Figure S16: Raw plots of XPS data for (a) Cu, (b) Fe, (c) Mn, (d) Ti and (e) Ni for NCFM, NCFMT and NCNFMT

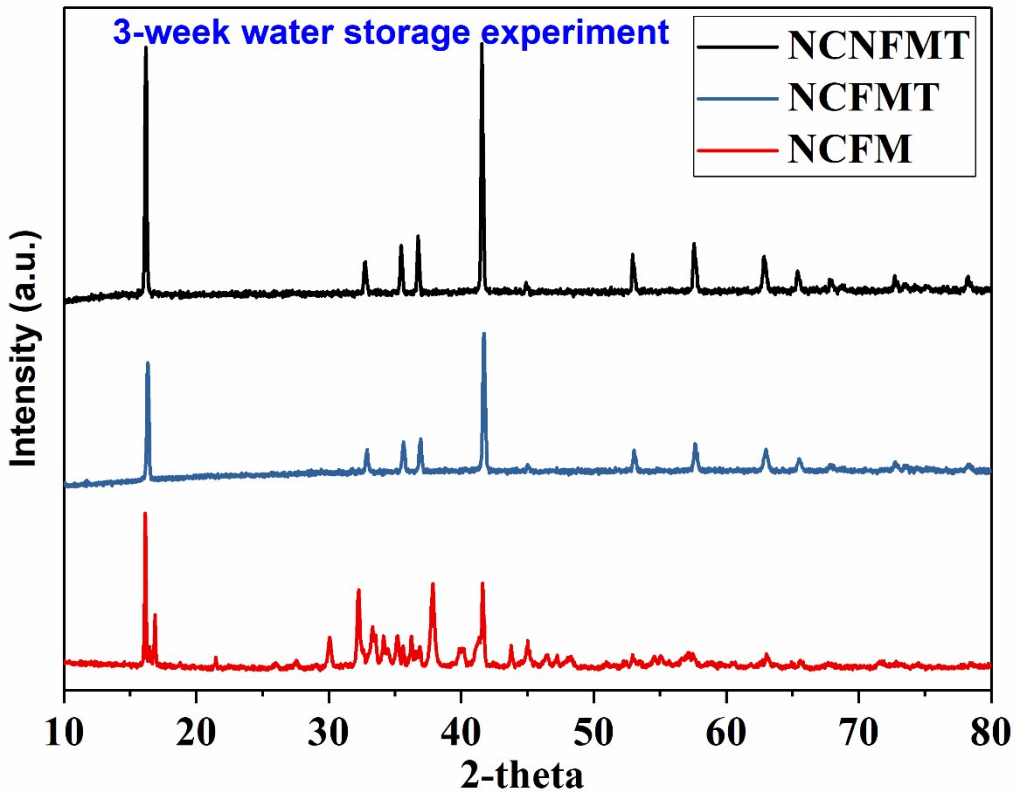

Figure S17: XRD plot after water-storage experiment for 3 week. NCFM, NCFMT and NCNFMT powder was stored in water for 3 weeks, then water was removed by evaporation at 60 ˚C followed by XRD measurement.

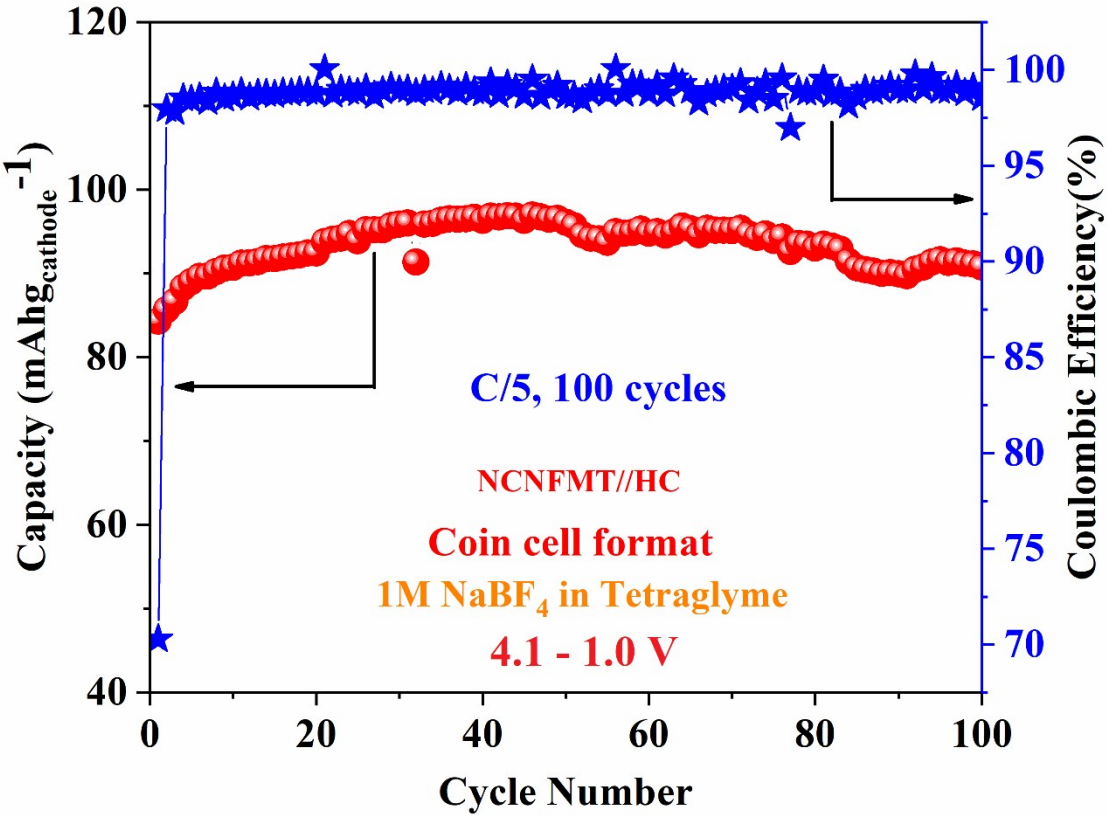

Figure S18: Cycling data of NCNFMT full cells in 2016 coin cell format.

Tables

Table 1: Rietveld Refinement parameters of powder-XRD. *-refined variables

NCFM Rietveld Refinement					
Spacegroup	R -3 m (166)				
R_w	6.1%	**GOF**	**0.12**		
a(Å)	2.94794(8)*				
c(Å)	16.4574(9)*				
Atom	**x**	**y**	**z**	**Occ**	**Beq**
Cu	0	0	0	0.22	1
Mn	0	0	0	0.48	1
Fe	0	0	0	0.3	1
Na	0	0	0.5	0.88(5)*	1
O	0	0	0.27229(15)*	1	1
NCFMT Rietveld Refinement					
Spacegroup	R -3 m (166)				
R_w	6.1%	**GOF**	**0.11**		
a(Å)	2.95609(8)*				
c(Å)	16.4589(9)*				
Atom	**x**	**y**	**z**	**Occ**	**Beq**
Cu	0	0	0	0.22	1
Mn	0	0	0	0.43	1
Ti	0	0	0	0.05	1
Fe	0	0	0	0.3	1
Na	0	0	0.5	0.86(5)*	1
O	0	0	0.27257(15)*	1	1
NCNFMT Rietveld Refinement					
Spacegroup	R -3 m (166)				
R_w	5.2%	**GOF**	**0.10**		
a(Å)	2.94833(8)*				
c(Å)	16.43893(8)*				
Atom	**x**	**y**	**z**	**Occ**	**Beq**
Cu	0	0	0	0.12	1
Mn	0	0	0	0.43	1
Ti	0	0	0	0.05	1
Ni	0	0	0	0.1	1
Fe	0	0	0	0.3	1
Na	0	0	0.5	0.88(5)*	1
O	0	0	0.27058(16)*	1	1

Table S2: Statistical data for EXAFS fitting

Sample	Path	R(Å)	σ^2 (X10^{-3} Å^2)	ΔE (eV)	R-factor	S_O^2	C.No.
NCFM							
Pristine	**Mn-O**	1.93(2)	1.68(3)	1.2(1)	0.041	0.51	5.5(1)
Desodiated_To_3.8V	**Mn-O**	1.92(2)	1.26(3)	1.0(1)	0.031	0.51	5.6(1)
Desodiated_To_4.1V	**Mn-O**	1.92(2)	2.6(3)	0.8(1)	0.037	0.51	5.8(1)
Sodiated_To_2.5V	**Mn-O**	1.93(2)	1.61(3)	0.9(1)	0.037	0.51	5.5(1)
Pristine	**Fe-O**	2.09(2)	4.22(3)	-0.04(2)	0.028	0.63	6.1(1)
Desodiated_To_3.8V	**Fe-O**	1.95(2)	8.85(3)	-1.98(2)	0.027	0.63	6.1(1)
Desodiated_To_4.1V	**Fe-O**	1.94(2)	10.5(3)	-0.5(1)	0.033	0.63	5.8(1)
Sodiated_To_2.5V	**Fe-O**	2.01(2)	4.75(3)	0.1(1)	0.011	0.63	6.2(1)
Pristine	**Cu-O**	2.30(1)	2.43(3)	-2.9(1)	0.019	0.87	2(f)
	Cu-O	2.00(1)	7.23(3)				4(f)
	Cu-TM	2.91(2)	5.89(3)				6(f)
Desodiated_To_3.8V	**Cu-O**	2.22(1)	3.57(2)	-8.3(1)	0.031	0.87	2(f)
	Cu-O	1.93(2)	7.90(2)				4(f)
	Cu-TM	2.85(2)	6.32(3)				6(f)
Desodiated_To_4.1V	**Cu-O**	2.17(1)	6.56(2)	-9.8(1)	0.038	0.87	2(f)
	Cu-O	1.90(2)	6.80(3)				4(f)
	Cu-TM	2.88(2)	7.59(3)				6(f)
Sodiated_To_2.5V	**Cu-O**	2.23(1)	7.49(2)	-6.0(1)	0.027	0.87	2(f)
	Cu-O	1.91(1)	7.52(3)				4(f)
	Cu-TM	2.90(2)	6.31(3)				6(f)
NCFMT							
Pristine	**Mn-O**	1.92(2)	1.77(3)	-0.1(1)	0.019	0.51	6.2(1)
Desodiated_To_3.8V	**Mn-O**	1.92(2)	1.42(3)	0.7(1)	0.031	0.51	5.9(1)
Desodiated_To_4.1V	**Mn-O**	1.91(2)	2.66(3)	0.5(1)	0.034	0.51	6.1(1)
Sodiated_To_2.5V	**Mn-O**	1.92(2)	1.51(3)	-0.3(1)	0.018	0.51	6.1(1)
Pristine	**Fe-O**	2.00(2)	5.93(3)	-0.1(1)	0.003	0.63	6.6(1)
Desodiated_To_3.8V	**Fe-O**	1.96(2)	8.55(3)	-1.7(1)	0.018	0.63	6.3(1)
Desodiated_To_4.1V	**Fe-O**	1.94(2)	10.51(3)	-1.6(1)	0.037	0.63	6(1)
Sodiated_To_2.5V	**Fe-O**	2.00(2)	5.88(3)	-0.3(1)	0.004	0.63	6.6(1)
Pristine	**Cu-O**	2.29(1)	2.92(2)	-4.8(1)	0.026	0.87	2(f)
	Cu-O	1.98(2)	7.55(3)				4(f)
	Cu-TM	2.89(2)	6.39(3)				6(f)
Desodiated_To_3.8V	**Cu-O**	2.26(1)	5.06(2)	-6.6(1)	0.033	0.87	2(f)
	Cu-O	1.94(2)	8.90(3)				4(f)
	Cu-TM	2.86(2)	6.78(3)				6(f)
Desodiated_To_4.1V	**Cu-O**	2.29(1)	4.93(2)	-3.2(1)	0.006	0.87	2(f)
	Cu-O	1.95(2)	8.24(3)				4(f)
	Cu-TM	2.88(2)	9.14(3)				6(f)
Sodiated_To_2.5V	**Cu-O**	2.30(2)	6.52(2)	-4.2(1)	0.024	0.87	2(f)
	Cu-O	1.99(2)	8.03(3)				4(f)
	Cu-TM	2.90(2)	6.83(3)				6(f)

NCNFMT							
Pristine	**Mn-O**	1.93(2)	0.17(3)	-3.0(1)	0.03547	0.51	5.5(1)
Desodiated_To_3.8V	**Mn-O**	1.88(2)	0.06(3)	-5.5(1)	0.024	0.51	5.7(1)
Desodiated_To_4.1V	**Mn-O**	1.90(2)	1.46(3)	-6.2(1)	0.041	0.51	5.8(1)
Sodiated_To_2.5V	**Mn-O**	1.92(2)	0.84(3)	-1.8(1)	0.033	0.51	5.6(1)
Pristine	**Fe-O**	2.00(2)	6.94(3)	-1.8(1)	0.039	0.63	6.8(1)
Desodiated_To_3.8V	**Fe-O**	1.94(2)	9.99(3)	-2.7(1)	0.019	0.63	6.4(1)
Desodiated_To_4.1V	**Fe-O**	1.92(2)	11.06(3)	-2.7(1)	0.033	0.63	6.0(1)
Sodiated_To_2.5V	**Fe-O**	2.00(2)	5.85(3)	-0.1(1)	0.003	0.63	6.1(1)
Pristine	**Ni-O**	2.04(2)	4.62(3)	-2.6(1)	0.014	0.75	6.0(1)
Desodiated_To_3.8V	**Ni-O**	1.91(2)	8.78(3)	-5.2(1)	0.018	0.75	5.6(1)
Desodiated_To_4.1V	**Ni-O**	1.89(2)	3.81(3)	-4.8(1)	0.032	0.75	5.1(1)
Sodiated_To_2.5V	**Ni-O**	2.07(2)	5.2(3)	-0.3(1)	0.027	0.75	6.1(1)
Pristine	**Cu-O**	2.30(2)	1.27(3)	-3.7(1)	0.023	0.87	2(f)
	Cu-O	2.00(2)	5.96(3)				4(f)
	Cu-TM	2.91(2)	5.60(3)				6(f)
Desodiated_To_3.8V	**Cu-O**	2.28(1)	2.57(3)	-3.7(1)	0.021	0.87	2(f)
	Cu-O	1.98(2)	8.06(3)				4(f)
	Cu-TM	2.89(2)	7.28(3)				6(f)
Desodiated_To_4.1V	**Cu-O**	2.22(1)	5.36(3)	-6.4(1)	0.005	0.87	2(f)
	Cu-O	1.95(2)	8.35(3)				4(f)
	Cu-TM	2.86(2)	8.64(3)				6(f)
Sodiated_To_2.5V	**Cu-O**	2.24(1)	7.38(2)	-2.8(1)	0.022	0.87	2(f)
	Cu-O	1.96(1)	8.98(2)				4(f)
	Cu-TM	2.91(2)	7.09(3)				6(f)

*S_o^2 was fixed from standard measurements, f = fixed.