Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

X-ray Absorption Near Edge Structure Simulation of $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$ via First-principles Calculation

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Table S1. Bader charge and atomic volume of Li1.0-NCM523 and Li0.5-NCM523

		Bader charge	Atomic volume(Å^3)
Li1.0	Ni^{2+}	8.85	8.63
	Ni^{3+}	8.79	7.86
Li/Ni	Ni^{2+}（Ni_{Li}）	8.80	8.80
Li0.5	Ni^{2+}	8.84	8.86
	Ni^{3+}	8.76	8.06
	Ni^{4+}	8.76	7.15
Li/Ni	Ni^{2+}（Ni_{Li}）	8.74	9.47

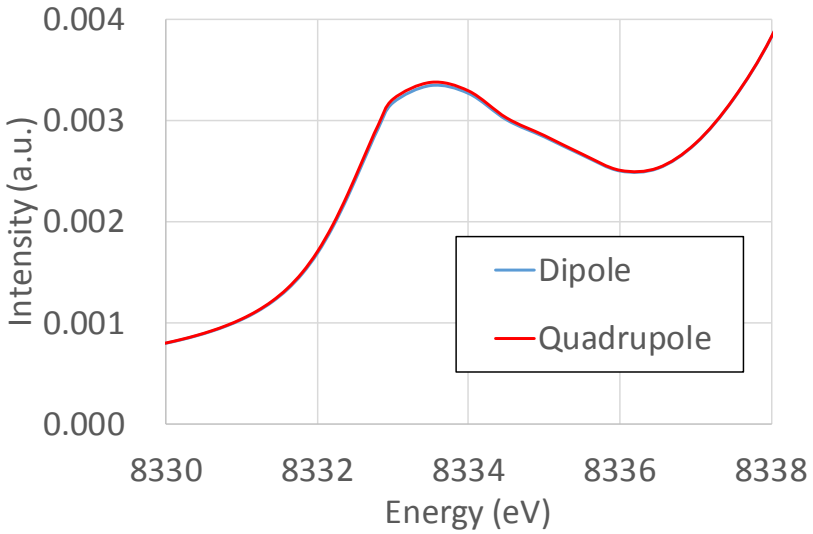

Fig. S1. Difference between quadrupole and dipole calculation at the Ni_{Li} pre-edge of Li0.5-NCM523.

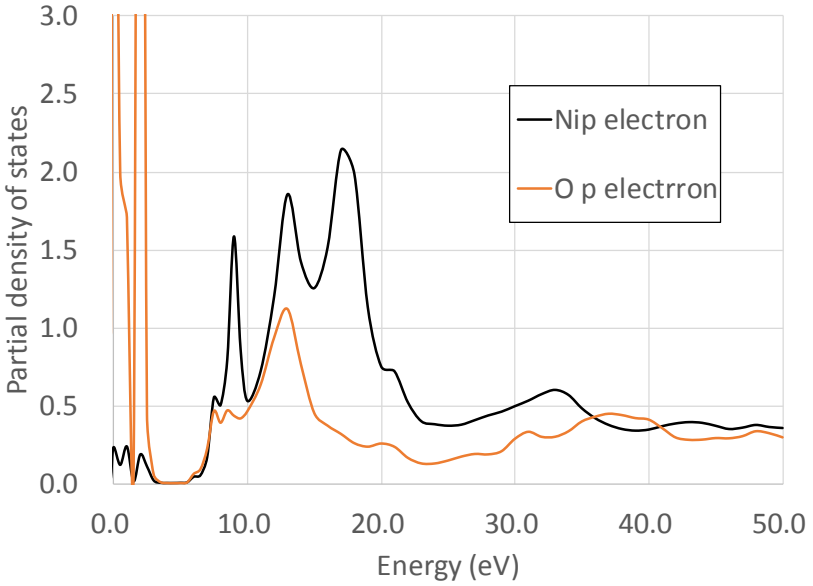

Fig. S2. Partial density of states of p electrons of N_{Li} of Li-0.5 NCM523. It can be understood that pre-edge peak is caused by hybridization of Ni p electrons with the nearest O p electrons.

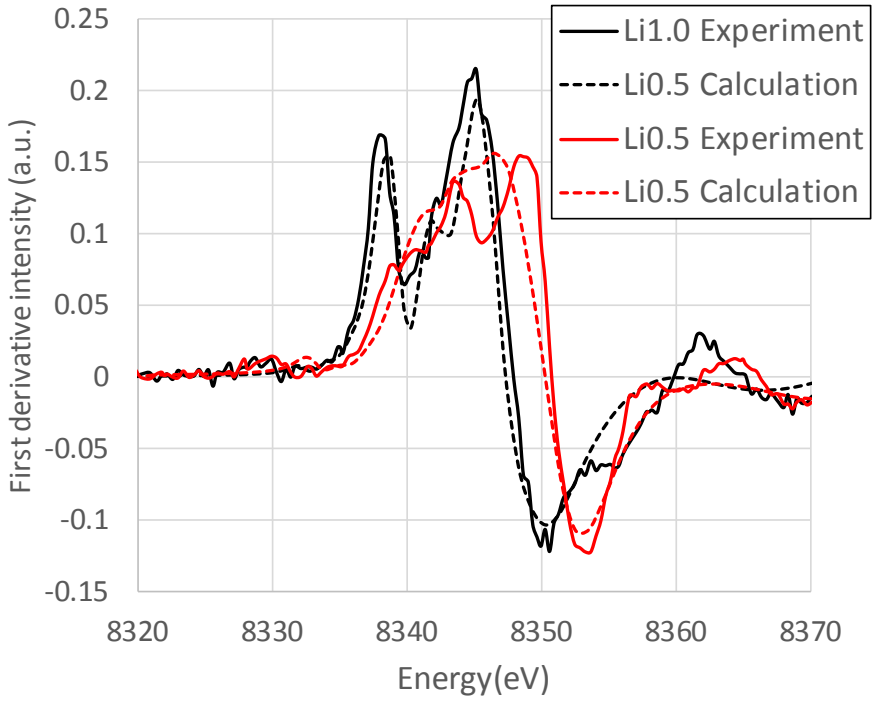

Fig. S3. First derivatives of XANES spectra in the Ni K-edge of Li-0.5 and Li-1.0 NCM523 via experiment and calculation.

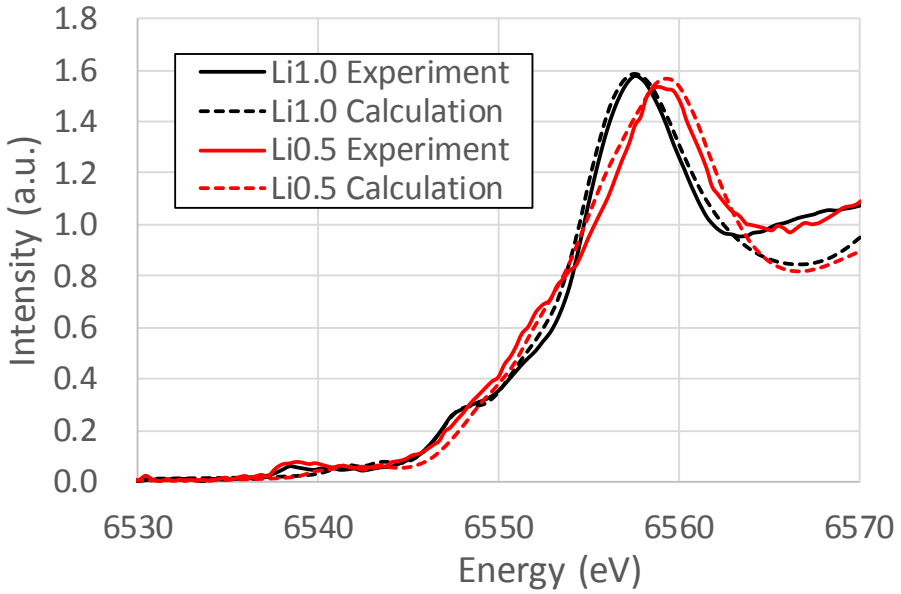

Fig. S4. XANES spectra of the Mn K-edge of Li-0.5 and Li-1.0 NCM523 via experiment and calculation.

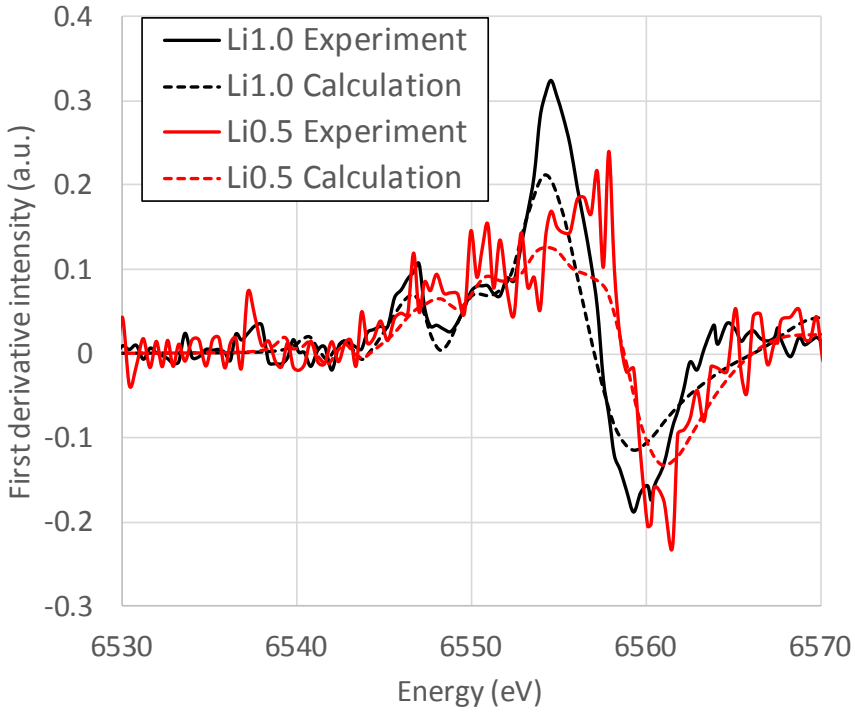

Fig. S5. First derivatives of XANES spectra in the Mn K-edge of Li-0.5 and Li-1.0 NCM523 via experiment and calculation.

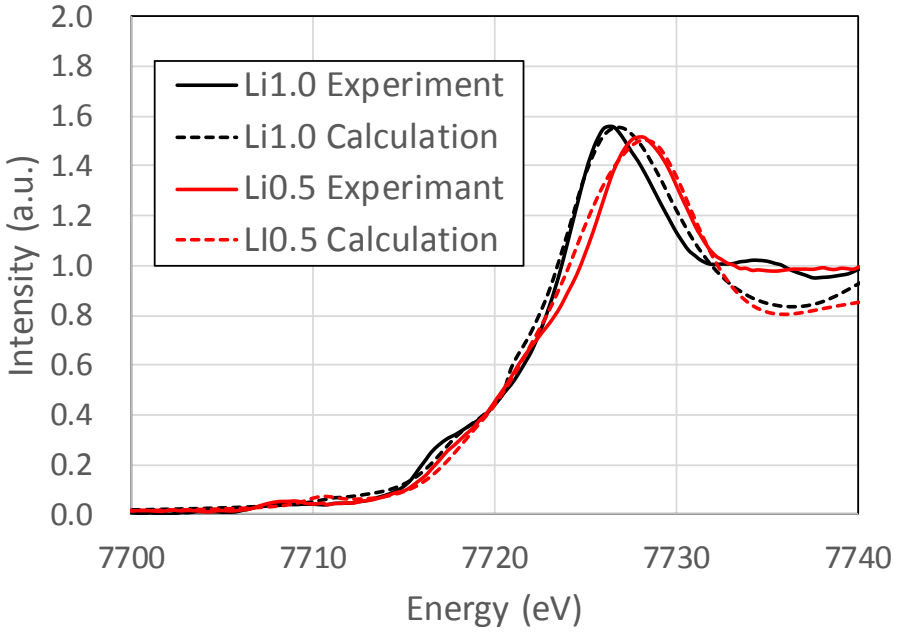

Fig. S6. XANES spectra of the Co K-edge of Li-0.5 and Li-1.0 NCM523 via experiment and calculation.

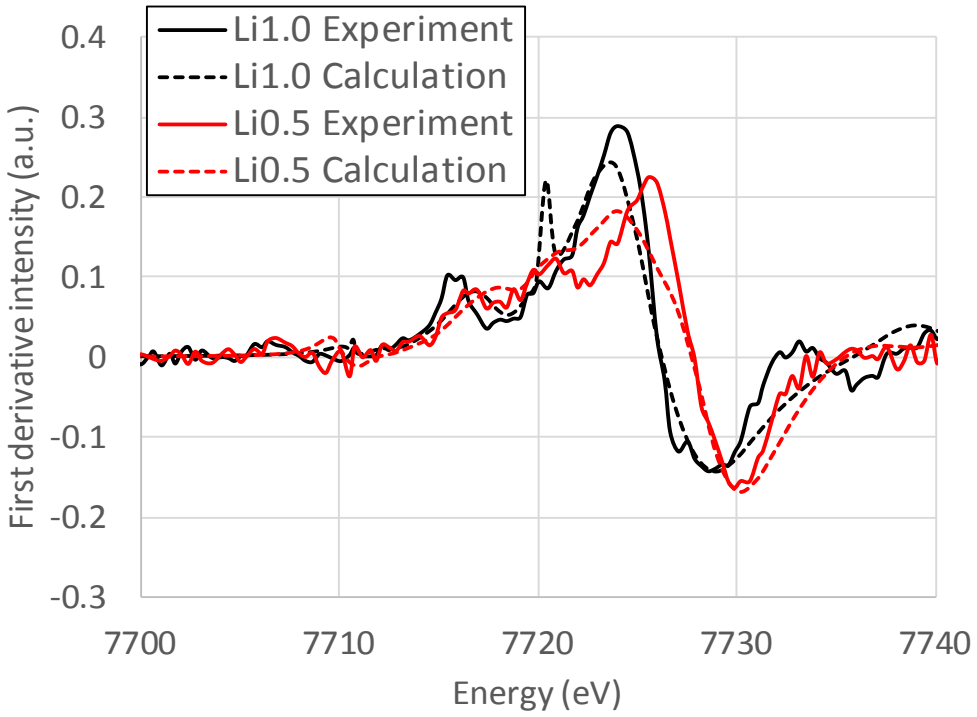

Fig. S7. First derivatives of XANES spectra in the Co K-edge of Li-0.5 and Li-1.0 NCM523 via experiment and calculation.

FDMNES input file for Li1.0

```
Absorber
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30

 Filout
  NiK

 Range
 -12. 0.2 0. 0.5 10. 1. 50.

Edge
K

 Radius                                7.0
Density
 state_all

Adimp
0.19
magnetism

Quadrupole

Atom_conf
11    1 4 5 11 14 17 18 21 25 26 28    1 3 2 4.5 3.5
19    2 3 6 7 8 9 10 12 13 15 16 19 20 22 23 24 27 29 30    1 3 2 5.0 3.0
12    31 32 33 34 35 36 37 38 39 40 41 42    1 3 2 3.5 3.5
18    43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 1 3 2 1.0 4.0

Hubbard
5.96 5.0 5.1
```

FDMNES input file for Li0.5

```
Absorber
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30

Filout
   NiK

 Range                                  ! Energy range of calculation (eV)
 -12. 0.2    0. 0.5 10. 1. 50.    ! first energy, step, intermediary energy, step ..., last energy

Edge
K

Radius                                  7.0

Density
  state_all

Adimp
0.19

magnetism

Quadrupole

Atom_conf
2      7 15     1 3 2 5.0 3.0
16    1 2 3 5 9 14 18 19 20 21 24 25 26 27 29 30     1 3 2 4.5 3.5
12    4 6 8 10 11 12 13 16 17 22 23 28 1 3 2 4.0 4.0
1      34     1 3 2     4.0 3.0
11    31 32 33 35 36 37 38 39 40 41 42     1 3 2 3.5 3.5
18    43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 1 3 2 1.0 4.0

Hubbard
5.96 5.0 5.1
```