Electronic Supplementary Material (ESI) For RSC Advances

Supporting Information for RSC Advances

Layered metal-organic framework based on tetracyanonickelate as cathode material for in situ Li-ion storage

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Calculation of the molecular formula of the as-prepared FF-PBAs

The nominal formula of PBAs is $K_xP[R(CN)_6]_{1-y}\cdot\square_y$. Therefore, we assumed the nominal formula of FF-PBAs as $K_xP[R(CN)_4]_{1-y}\cdot$ (where P: N-coordinated transition metal ions; R: C-coordinated transition metal ions;). Furthermore, we normalized the transition metal ion P as 1, i.e., $K_xP_1[R(CN)_4]_{1-y}$. Thus, another transition metal ion R was calculated based on the quantitative measurements by XRF (Table S1). The elemental mass ratio in each FF-PBA was obtained as follows:

Stoichiometric number of Ni:

Ni (mass%)/P ion (mass %) = A (the elemental mass% in the $K_xP_1[R(CN)_4]_{1-y}\cdot\square_y$) (1)

Stoichiometric number of K ion:

K (mass%)/P ion (mass%) = B (the elemental mass% in the $K_xP_1[R(CN)_4]_{1-y}\cdot\square_y$) (2)

Thus, the values of x and y in the molecular formula can be calculated.

Table S1. Elemental mass ratio of each sample measured by XRF.

Sample	Ni (mass%)	P ion (mass%)	C (mass%)	N (mass%)	K (mass%)
Ni/Ni	23.80	—	11.80	17.70	4.56
Ni/Fe^{3+}	10.70	8.06	13.00	17.30	1.13
Ni/Co	0.60	0.67	8.36	6.81	0.09
Ni/Zn	1.93	1.51	13.40	15.90	0.11
Ni/Mn	8.95	10.40	14.90	21.40	0.35
Ni/Cu	12.30	14.40	14.70	23.70	2.08
Ni/Fe^{2+}	4.50	5.48	13.50	16.20	0.36

Note: The mass% values in this table represent each elemental mass% based on the total weight of the pretreated sample for XRF measurement.

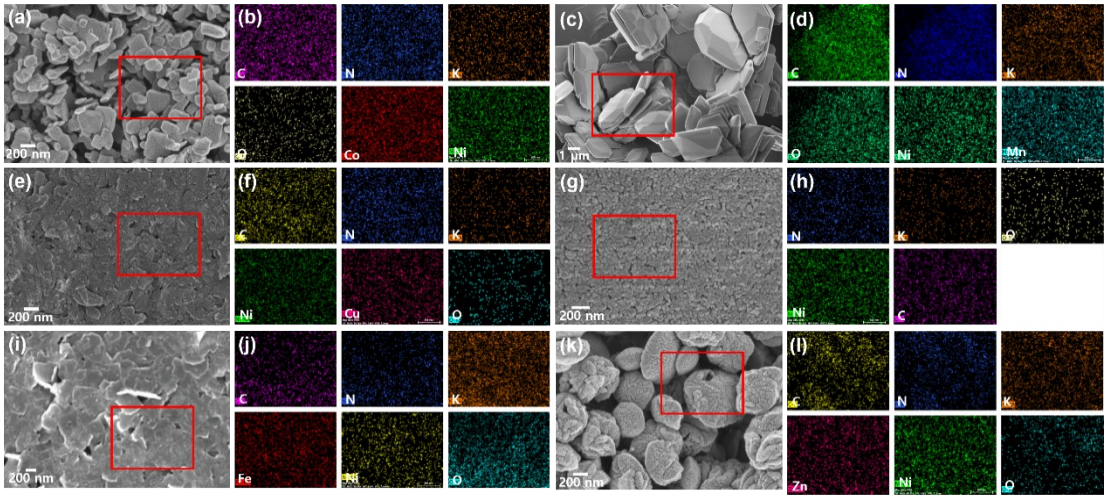

Fig. S1. SEM and EDX elemental mappings of as-prepared (a, b) Ni/Co, (c, d) Ni/Mn, (e, f) Ni/Cu, (g, h) Ni/Ni, (i, j) Ni/Fe^{3+}, and (k, l) Ni/Zn.

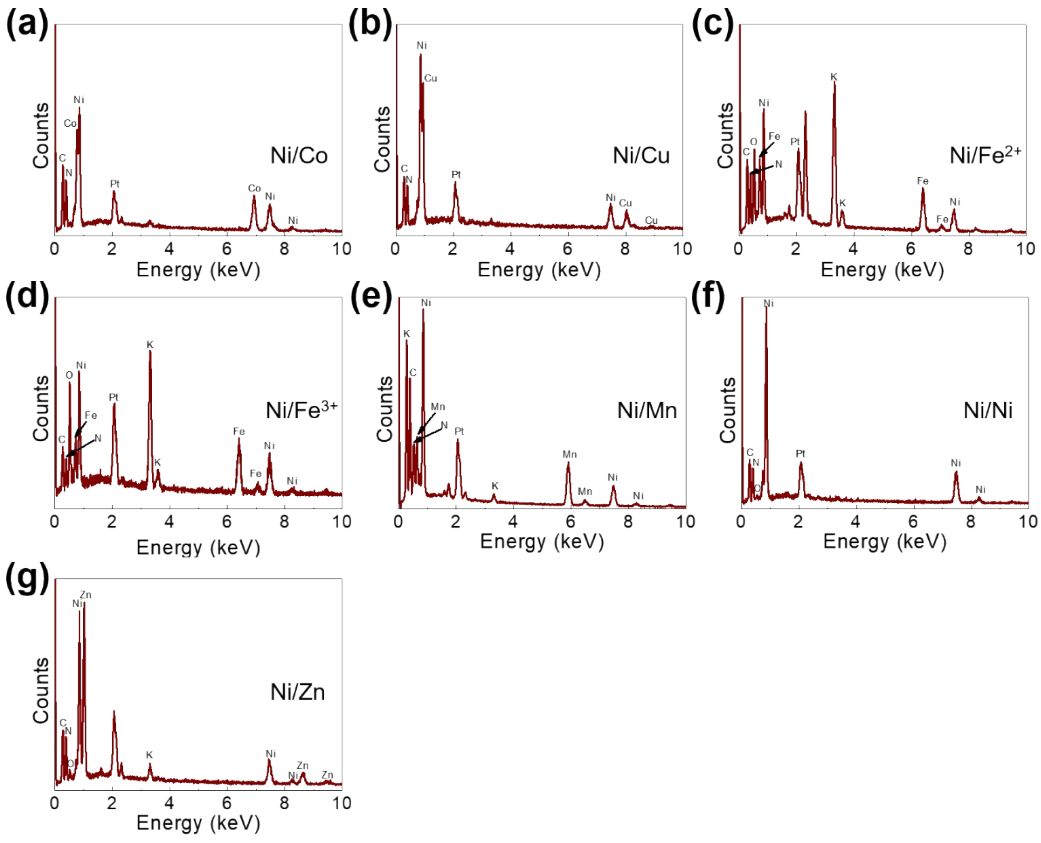

Fig. S2. EDX elemental spectra of (a) Ni/Co, (b) Ni/Cu, (c) Ni/Fe^{2+}, (d) Ni/Fe^{3+}, (e) Ni/Mn, (f) Ni/Ni, and (g) Ni/Zn.

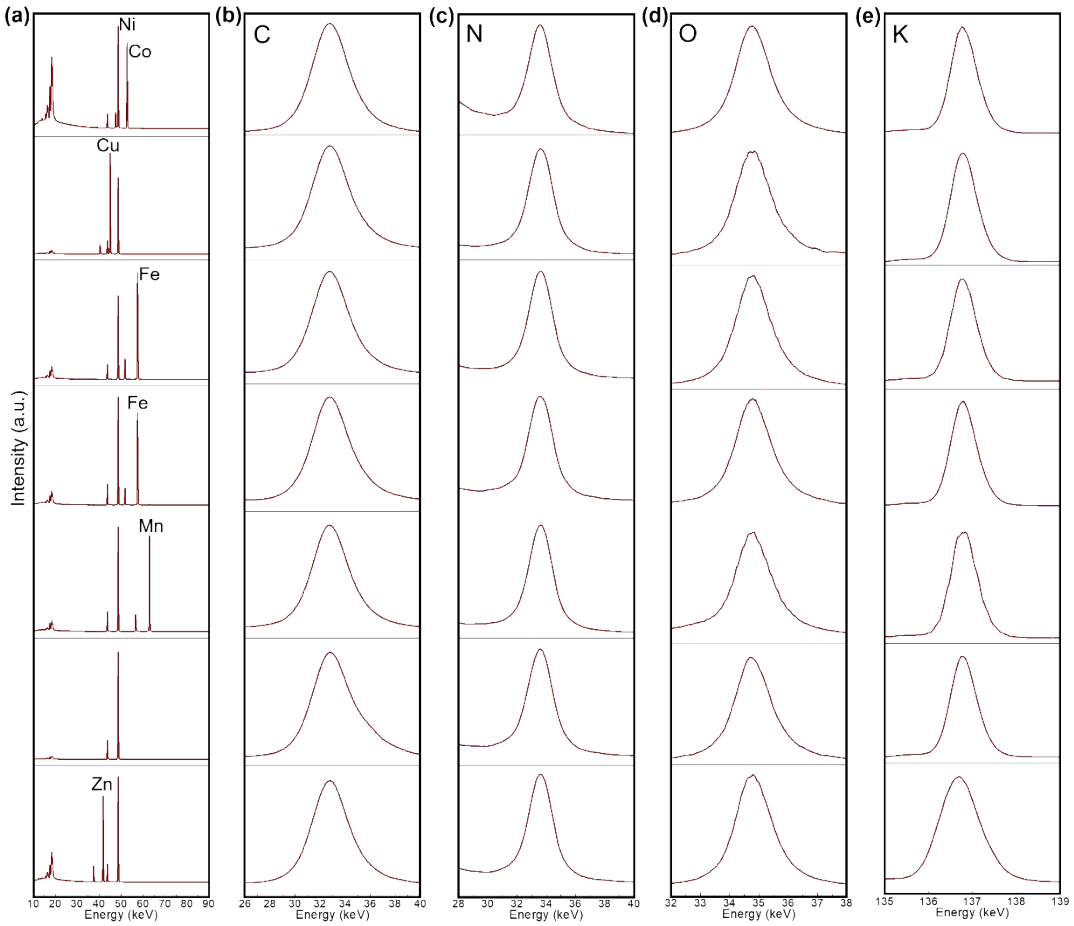

Fig. S3. XRF of (a) wide survey, (b) C, (c) N, (d) O, and (e) K for Ni/Co, Ni/Cu, Ni/Fe^{2+}, NiFe^{3+}, Ni/Mn, Ni/Ni, and Ni/Zn (from top to bottom).

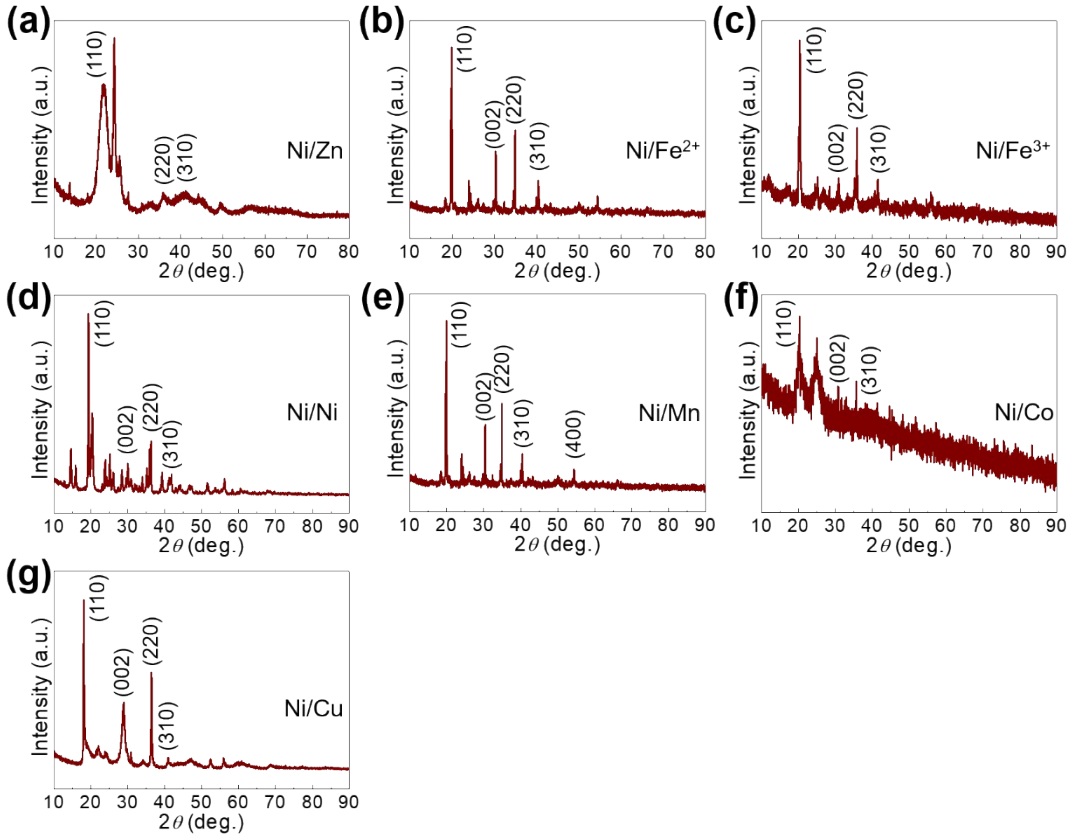

Fig. S4. XRD spectra of the as-prepared (a) Ni/Zn, (b) Ni/Fe^{2+}, (c) Ni/Fe^{3+}, (d) Ni/Ni, (e) Ni/Mn, (f) Ni/Co, and (g) Ni/Cu.

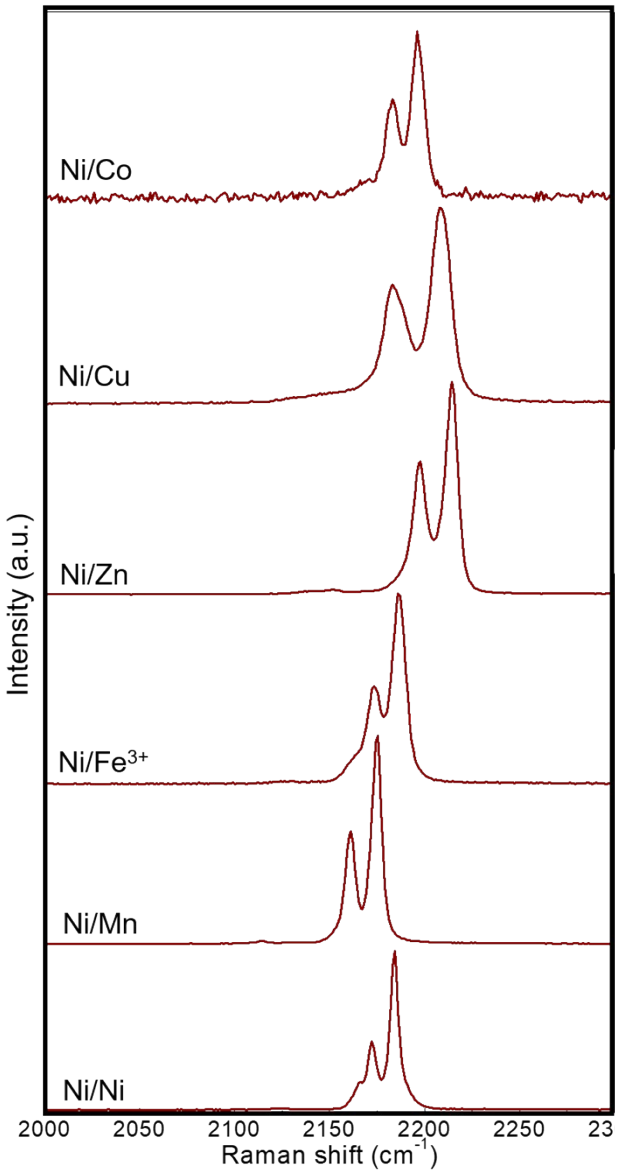

Fig. S5. Raman spectra of the as-prepared FF-PBAs.

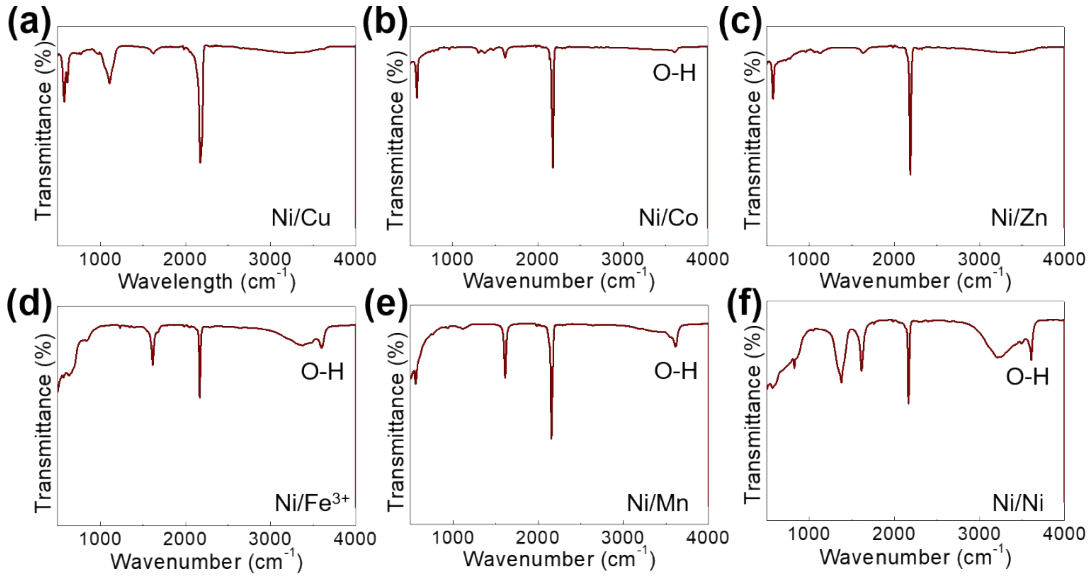

Fig. S6. FT-IR spectra of (a) Ni/Cu, (b) Ni/Co, (c) Ni/Zn, (d) Ni/Fe^{3+}, (e) Ni/Mn, and (f) Ni/Ni.

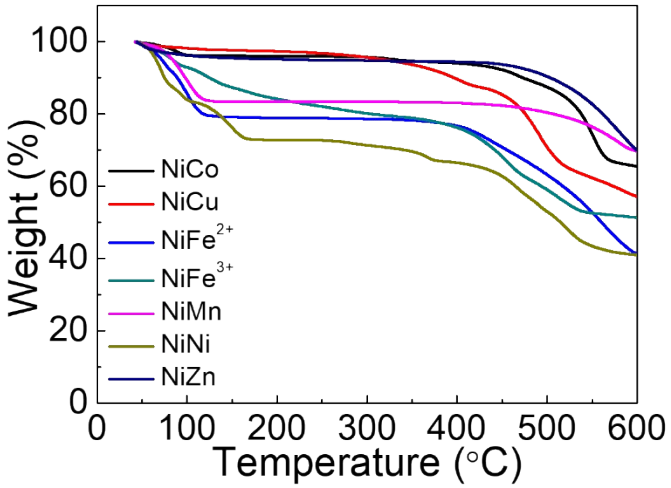

Fig. S7. TGA curves of the FF-PBAs.

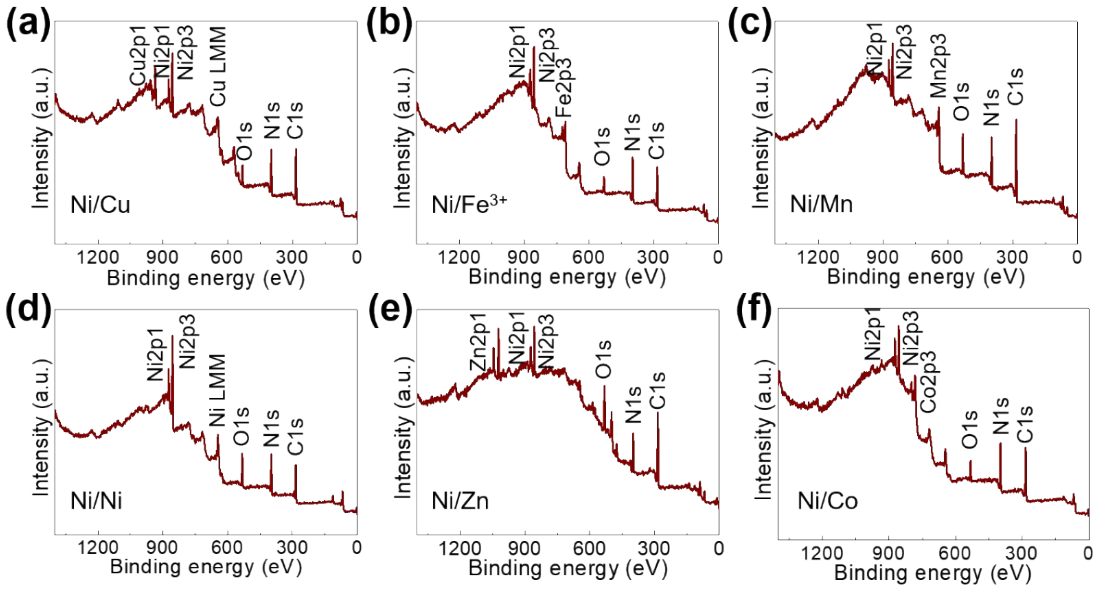

Fig. S8. Wide survey of XPS for (a) Ni/Cu, (b) Ni/Fe^{3+}, (c) Ni/Mn, (d) Ni/Ni, (e) Ni/Zn, and (f) Ni/Co.

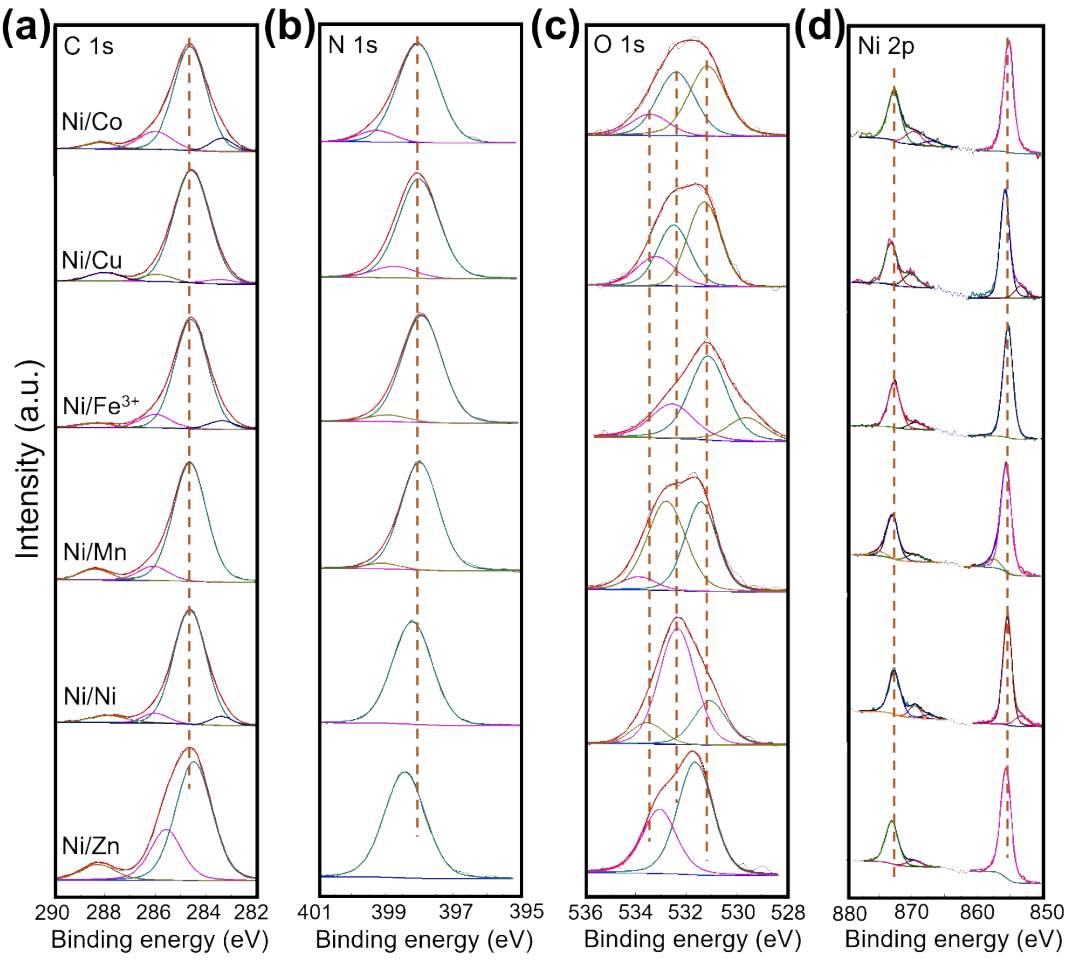

Fig. S9. Deconvoluted XPS of (a) C 1s, (b) N 1s, (c) O 1s, and (d) Ni 2p for the FF-PBAs.

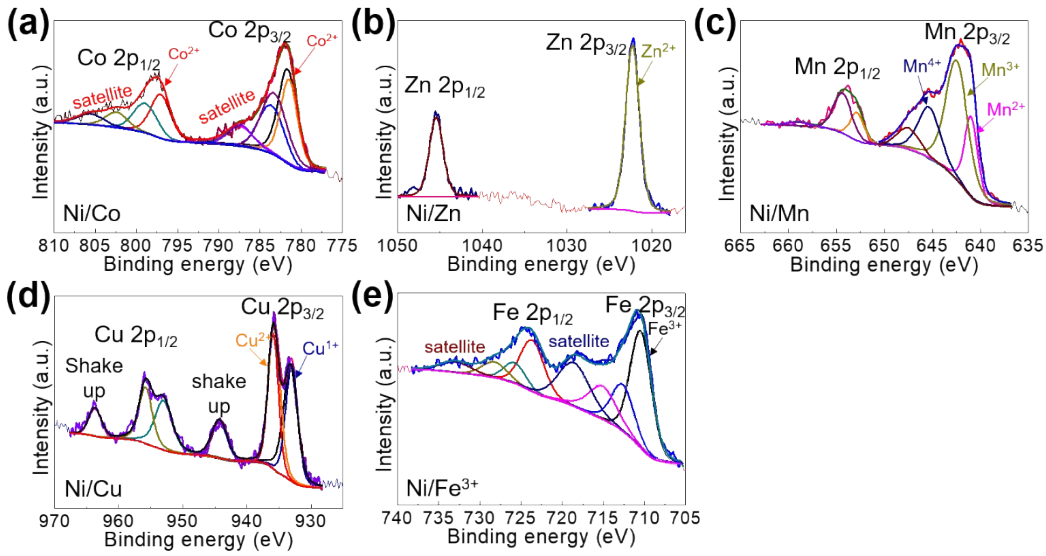

Fig. S10. Deconvoluted XPS of (a) Co 2p in Ni/Co, (b) Zn 2p in Ni/Zn, (c) Mn 2p in Ni/Mn, (d) Cu 2p in Ni/Cu, and (e) Fe 2p in Ni/Fe^{3+}.

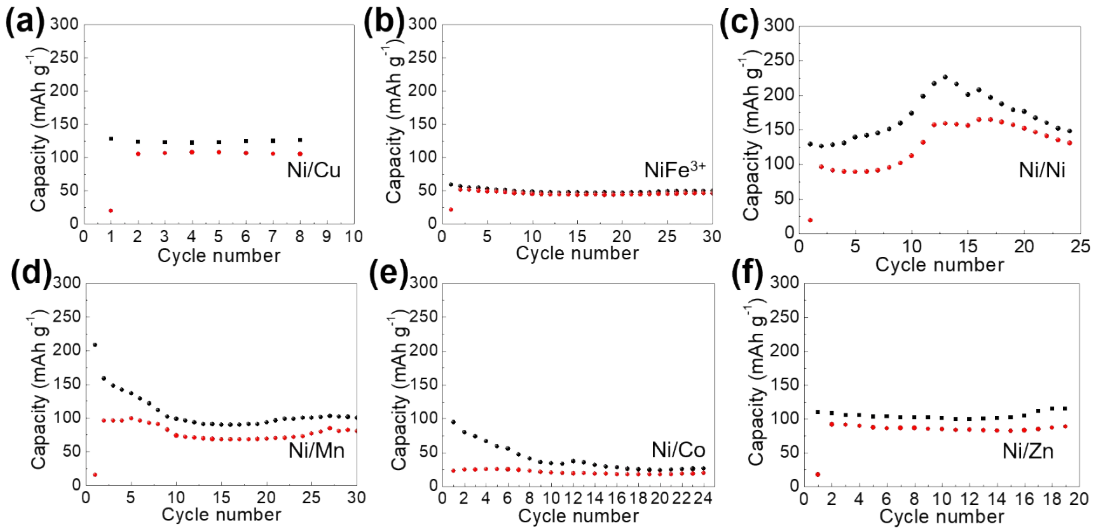

Fig. S11. Repeated charge/discharge cycling measurement at 100 mA g^{-1} for (a) Ni/Cu, (b) Ni/Fe^{3+}, (c) Ni/Ni, (d) Ni/Mn, (e) Ni/Co, (f) Ni/Zn, and (g) Ni/Fe^{2+} in half-cells, respectively, within a same potential window of 2.2–4.5 V versus Li^+/Li to demonstrate the electrochemical properties as cathode materials of LIBs.

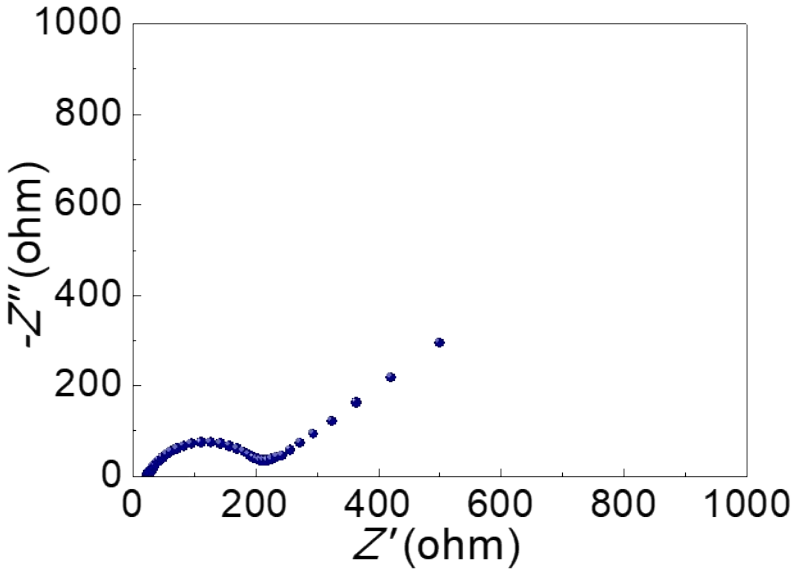

Fig. S12. EIS spectra of the Ni/Fe^{2+} electrode.