ARTICLE

Electronic Supporting Information (ESI)

Correlation of phase (in)stability and lattice misfits for high-power-density Na cathodes

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Table S1. Rietveld refinement parameters based on powder XRD data for NM13 and NM12, respectively.

Nominal Composition	**$Na_{0.62}Ni_{0.25}Mn_{0.75}O_2$ (NM13)**	**$Na_{0.67}Ni_{0.33}Mn_{0.67}O_2$ (NM12)**
a, Å	2.8866	2.8888
c, Å	11.2062	11.1527
Occupancy :		
Na_e	0.470	0.350
Na_f	0.192	0.230
Ni	0.243	0.333
Mn	0.757	0.667
Refined Composition	$Na_{0.662}Ni_{0.243}Mn_{0.757}O_2$	$Na_{0.70}Ni_{0.333}Mn_{0.667}O_2$
ICP-OES Composition	$Na_{0.640}Ni_{0.248}Mn_{0.738}O_2$	$Na_{0.73}Ni_{0.335}Mn_{0.695}O_2$

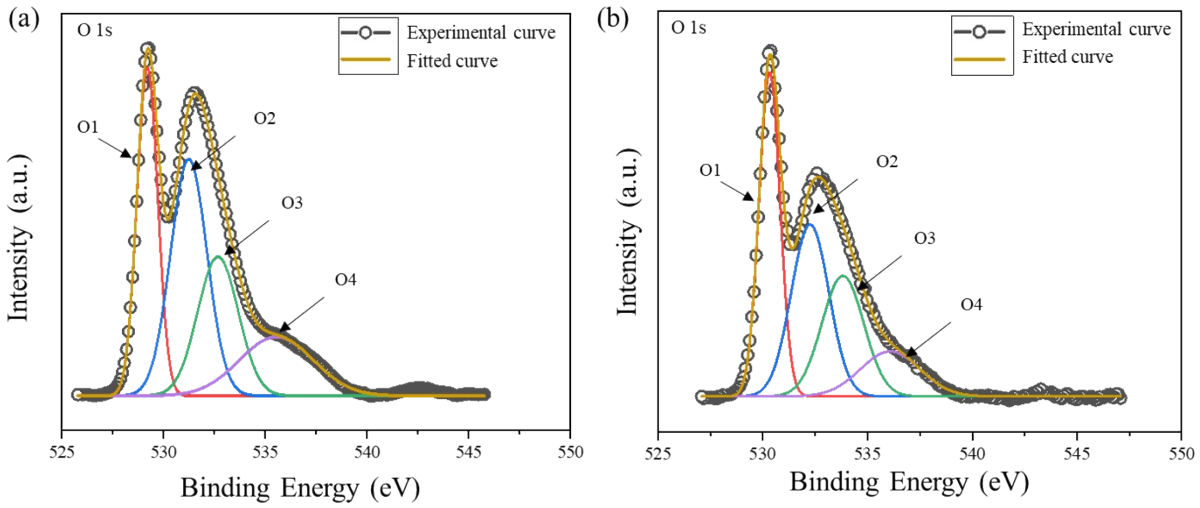

Figure S1. (a-b) XPS core level high-resolution spectra of O 1s of the NM12 and NM13, respectively.

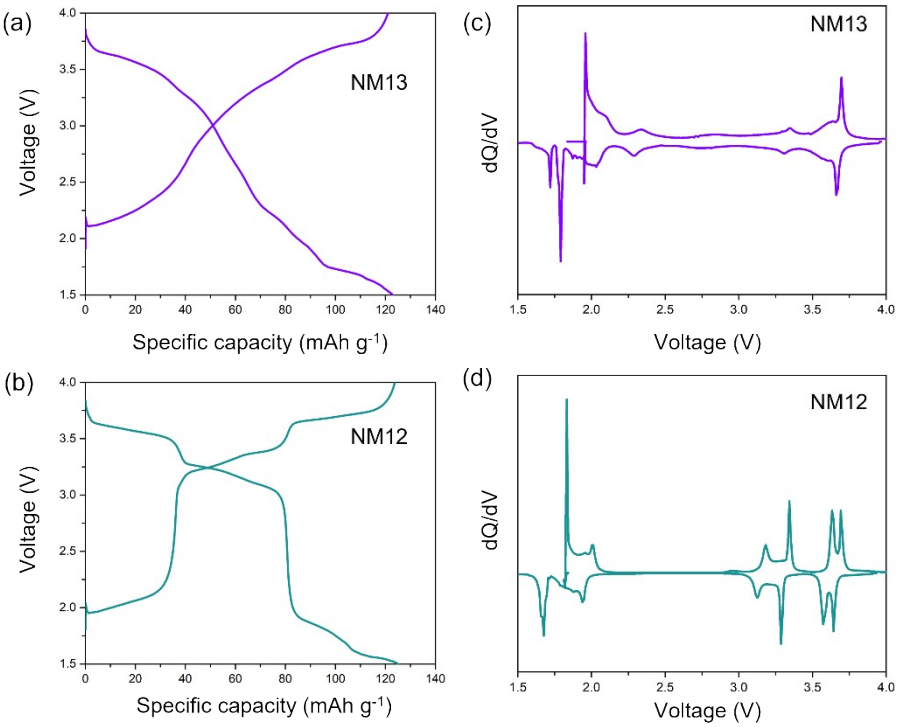

Figure S2. (a & b) Potential profiles of for $Na_{0.62}[Ni_{1/4}Mn_{3/4}]O_2$ and $Na_{0.67}[Ni_{1/3}Mn_{2/3}]O_2$ depending on voltage cut-off 1.5−4.0 V at current rate of 1 C. (c & d) Differential capacity of for NM13 and NM12 depending on voltage cut-off 1.5−4.0 V at current rate of 1 C.

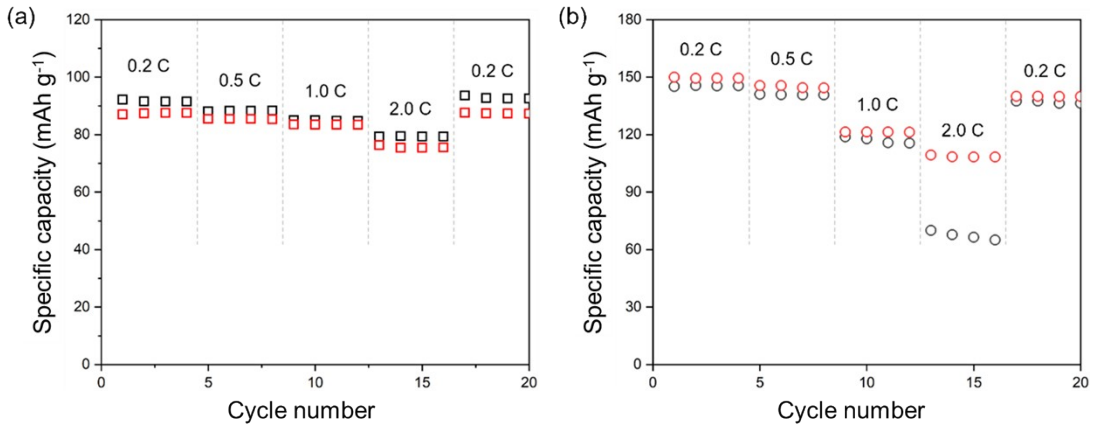

Figure S3. Rate capability performances of NM12 and NM13 depending on voltage cut-off (a) 2.0–4.0 V and (b) 1.5–4.0 V

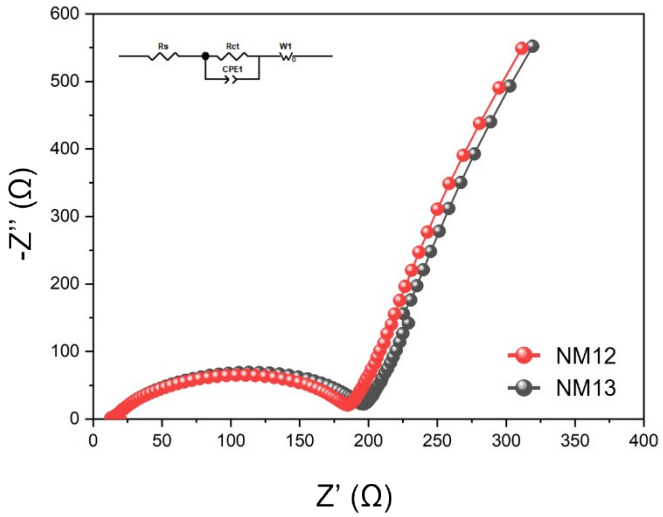

Figure S4. Electrochemical impedance spectrum of NM12 and NM13 cell before cycling. obtained in the frequency range from 100 kHz to 0.1 kHz. With the equivalent circuit of the EIS which consists of solution resistance (R_s), charge transfer resistance (R_{ct}), Warburg impedance (Z_w), and constant phase element (CPE)

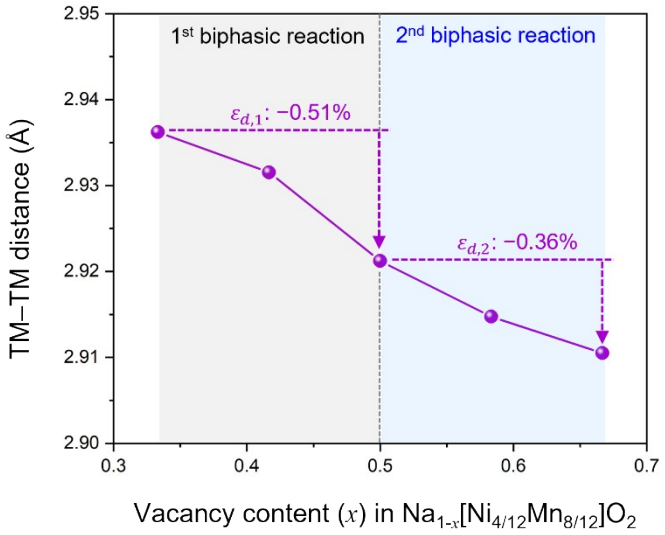

Figure S5. TM–TM distance, calculated by first principles calculations, as a function of vacancy content (x) in $Na_{1-x}[Ni_{4/12}Mn_{8/12}]O_2$.

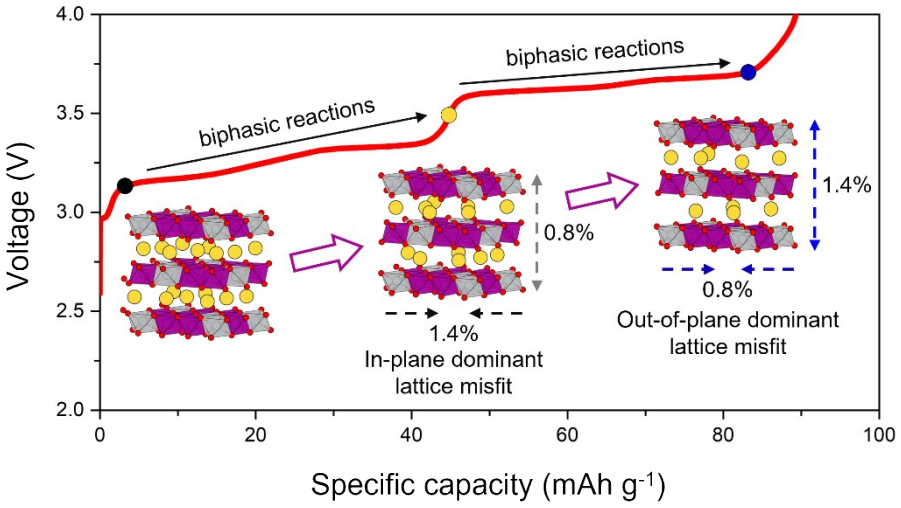

Figure S6. Galvanostatic charge curves of for $Na_{0.67}[Ni_{1/3}Mn_{2/3}]O_2$ depending on voltage cut-off 2.0–4.0 V at current rate of 1.0 C. Corresponding atomic models with lattice misfit are described in the inset figures.