

High-performance full sodium cells based on MgO-treated P2-type $\text{Na}_{0.67}(\text{Mn}_{0.5}\text{Fe}_{0.5})_{1-x}\text{Co}_x\text{O}_2$ cathodes

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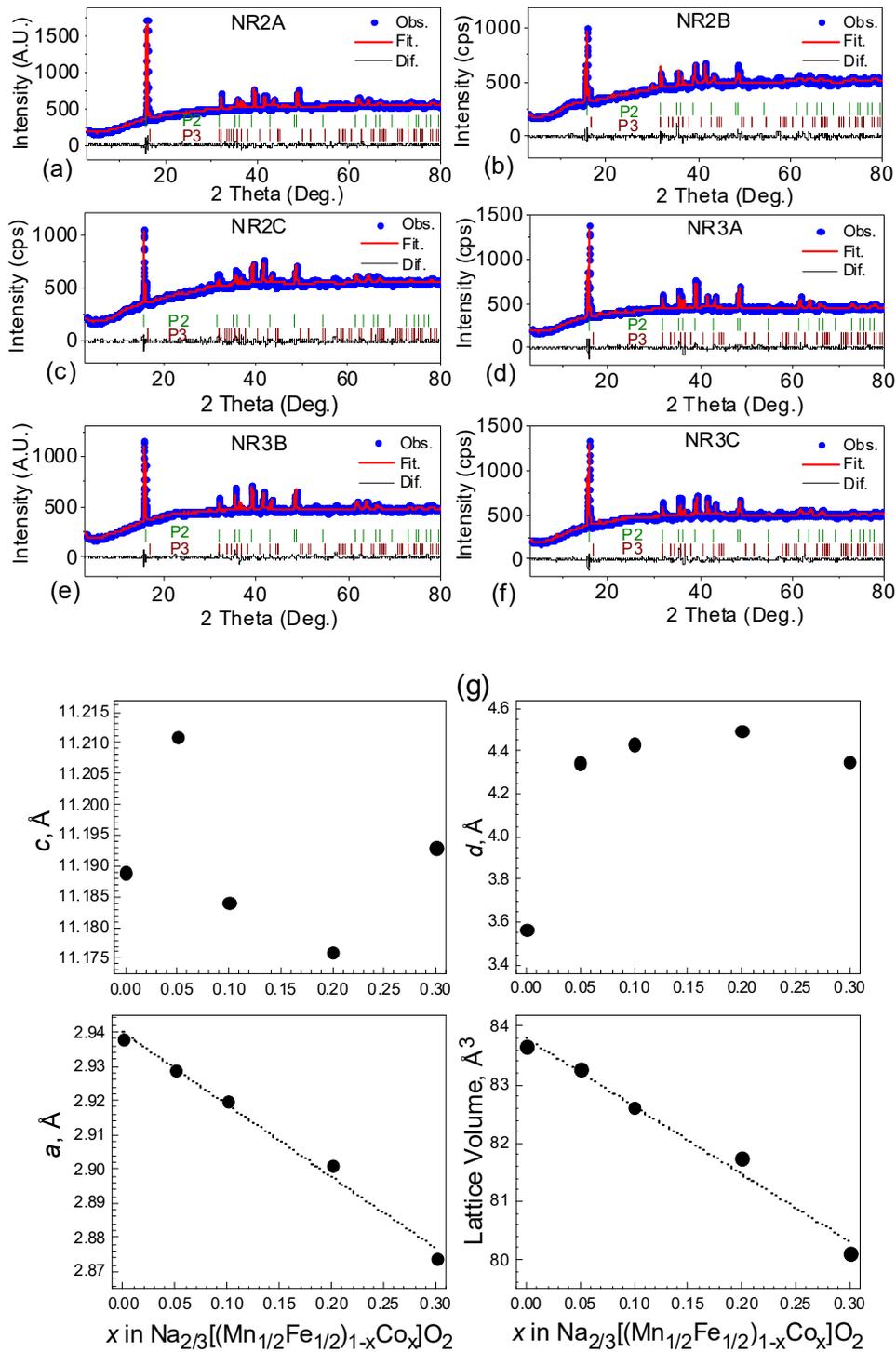


Figure S1: Rietveld-refined x-ray diffraction patterns (a) NR2A, (b) NR2B, (c) NR2C and (d)NR3A, (e)NR3B (f) NR3C, (g) the dependence of the lattice parameters (a, c, and volume) and the interlayer distance (denoted as d) of the P2-oxides on the Co content

Table S1. The calculated lattice parameters, Na-layer distance, and weighted R (wR%) factor for Co-doped and MgO-treated oxides.

| Sample Code | Phase | a (Å) | b (Å) | c (Å) | V(Å ³) | Na layer dist.(Å) | Phase Ratio % | wR % |
|----------------|-------|--------------|------------|-------------|--------------------|-------------------|---------------|------|
| P2 struc. [32] | P2 | 2.878 | | 11.163 | | 3.635 | - | - |
| P3 struc.* | P3 | 5.63 | 2.86 | 5.77 | 85.58 | | - | - |
| NR-0 | P2 | 2.938 (±3) | | 11.189 (±2) | 83.66 (±21) | 3.567 | - | 2.85 |
| NR-1 | P2 | 2.929 (±3) | | 11.211 (±1) | 83.27 (±18) | 4.345 | 99.87 | 2.76 |
| | P3 | 2.862 (±2) | 5.631 (±2) | 5.779 (±4) | 85.85 (±14) | | 0.13 | |
| NR-2 | P2 | 2.920 (±3) | | 11.184 (±2) | 82.61 (±21) | 4.434 | 99.56 | 3.15 |
| | P3 | 2.863 (±2) | 5.633 (±1) | 5.781 (±3) | 86.06 (±15) | | 0.44 | |
| NR-2A | P2 | 2.917 (±3) | | 11.210 (±1) | 82.61 (±17) | 4.438 | 98.15 | 2.58 |
| | P3 | 2.871 (±4) | 5.623 (±2) | 5.791 (±4) | 86.13 (±21) | | 1.85 | |
| NR-2B | P2 | 2.914 (±3) | | 11.184 (±2) | 82.28 (±20) | 4.367 | 97.73 | 2.38 |
| | P3 | 2.862 (±4) | 5.643 (±3) | 5.811 (±2) | 86.61 (±23) | | 2.27 | |
| NR-2C | P2 | 2.901 (±4) | | 11.208 (±2) | 82.18 (±27) | 4.296 | 98.36 | 2.59 |
| | P3 | 2.871 (±2) | 5.633 (±1) | 5.821 (±4) | 87.23 (±26) | | 1.64 | |
| NR-3 | P2 | 2.906 (±4) | | 11.176 (±2) | 81.74 (±22) | 4.497 | 99.35 | 2.73 |
| | P3 | 2.841 (±2) | 5.613 (±3) | 5.831 (±4) | 85.66 (±21) | | 0.65 | |
| NR-3A | P2 | 2.899 (±5) | | 11.166 (±3) | 81.29 (±32) | 4.317 | 97.98 | 3.23 |
| | P3 | 2.851 (±3) | 5.633 (±2) | 5.851 (±3) | 83.81 (±22) | | 2.02 | |
| NR-3B | P2 | 2.888 (±0.5) | | 11.253 (±4) | 81.28 (±32) | 4.432 | 98.44 | 2.71 |
| | P3 | 2.858 (±1) | 5.643 (±4) | 5.891 (±3) | 83.18 (±26) | | 1.56 | |
| NR-3C | P2 | 2.889 (±5) | | 11.208 (±3) | 81.02 (±29) | 4.291 | 96.53 | 2.49 |
| | P3 | 2.866 (±2) | 5.666 (±4) | 5.874 (±2) | 85.07 (±21) | | 3.47 | |
| NR-4 | P2 | 2.874 (±3) | | 11.193 (±7) | 80.11 (±10) | 4.349 | 98.93 | 2.84 |
| | P3 | 2.886 (±4) | 5.686 (±4) | 5.844 (±4) | 88.34 (±16) | | 1.07 | |

*

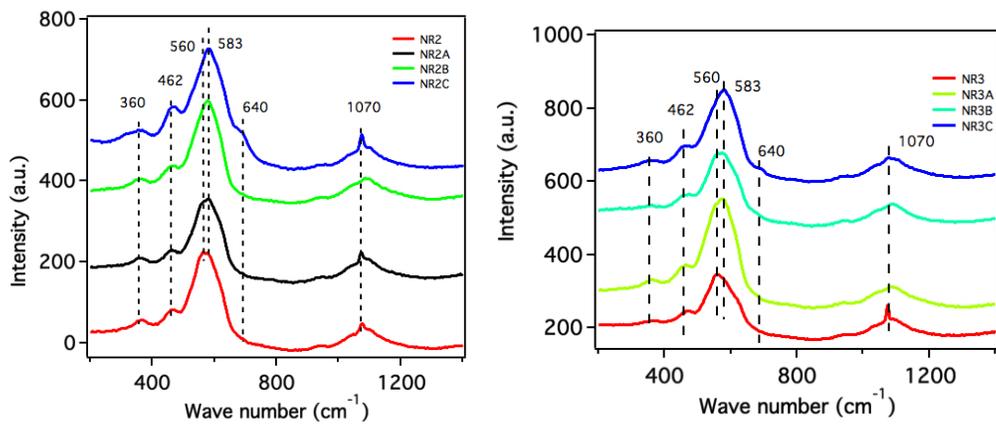
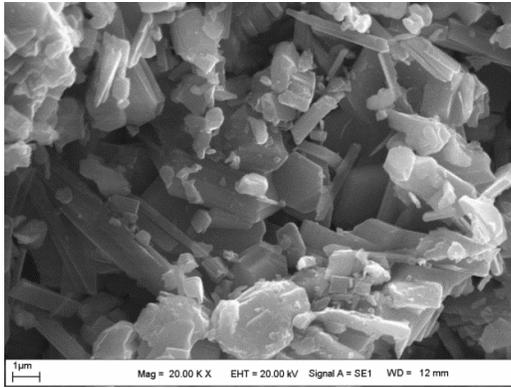
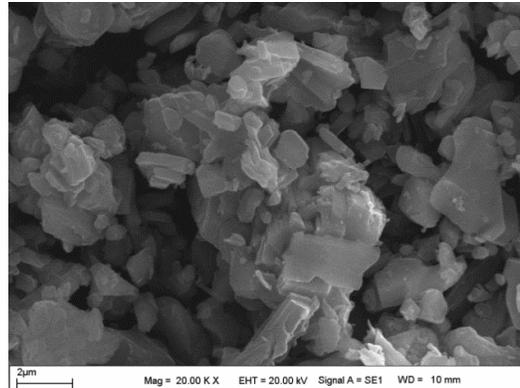


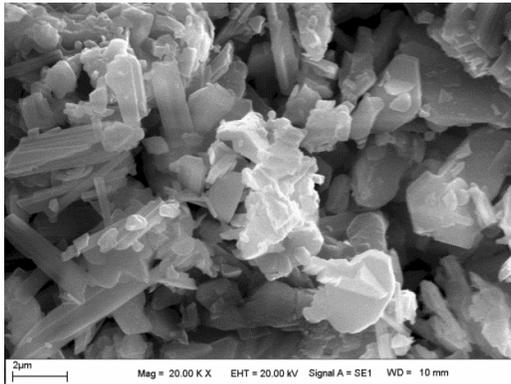
Figure S2. Raman Spectrum of the sample produced.



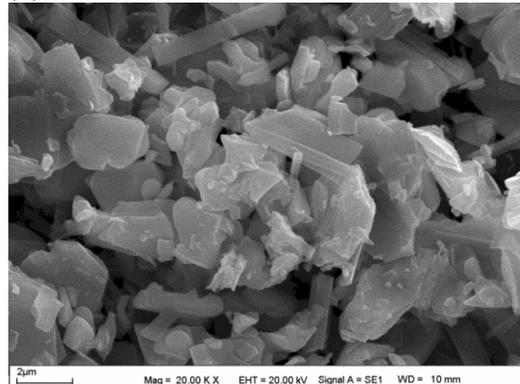
(a)



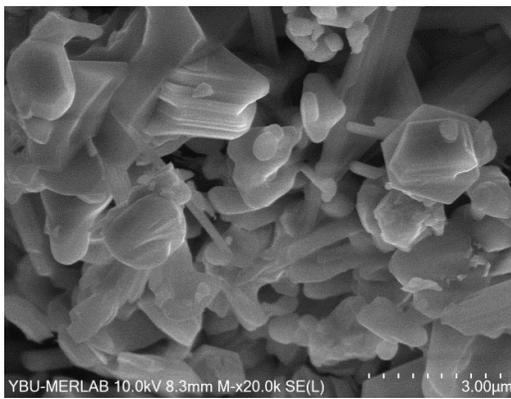
(b)



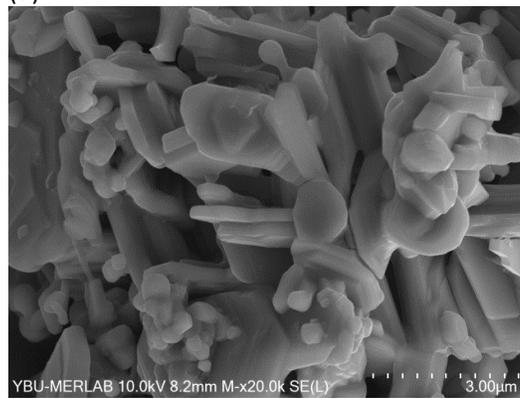
(c)



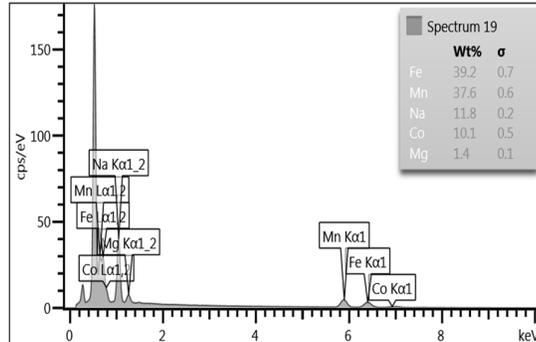
(d)



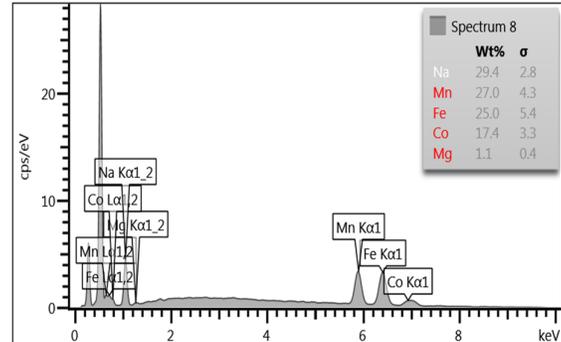
(e)



(f)



(g)



(h)

Figure S3. SEM images of (a) NR1, (b) NR2, (c) NR3, (d) NR4, (e)NR2B (f)NR3A, and EDX data of (g) NR2B and NR3A

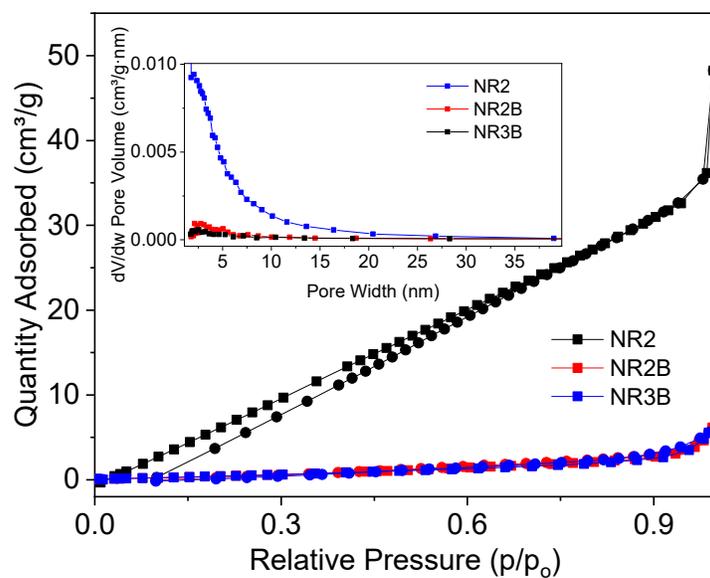


Figure S4. BET analysis results of NR2, NR2B and NR3B

Table S2. BET data of NR2, NR2B and NR3B

| Sample | BET surface area, m ² /g |
|--------|-------------------------------------|
| NR2 | 32.0 |
| NR2B | 2.4 |
| NR3B | 2.1 |

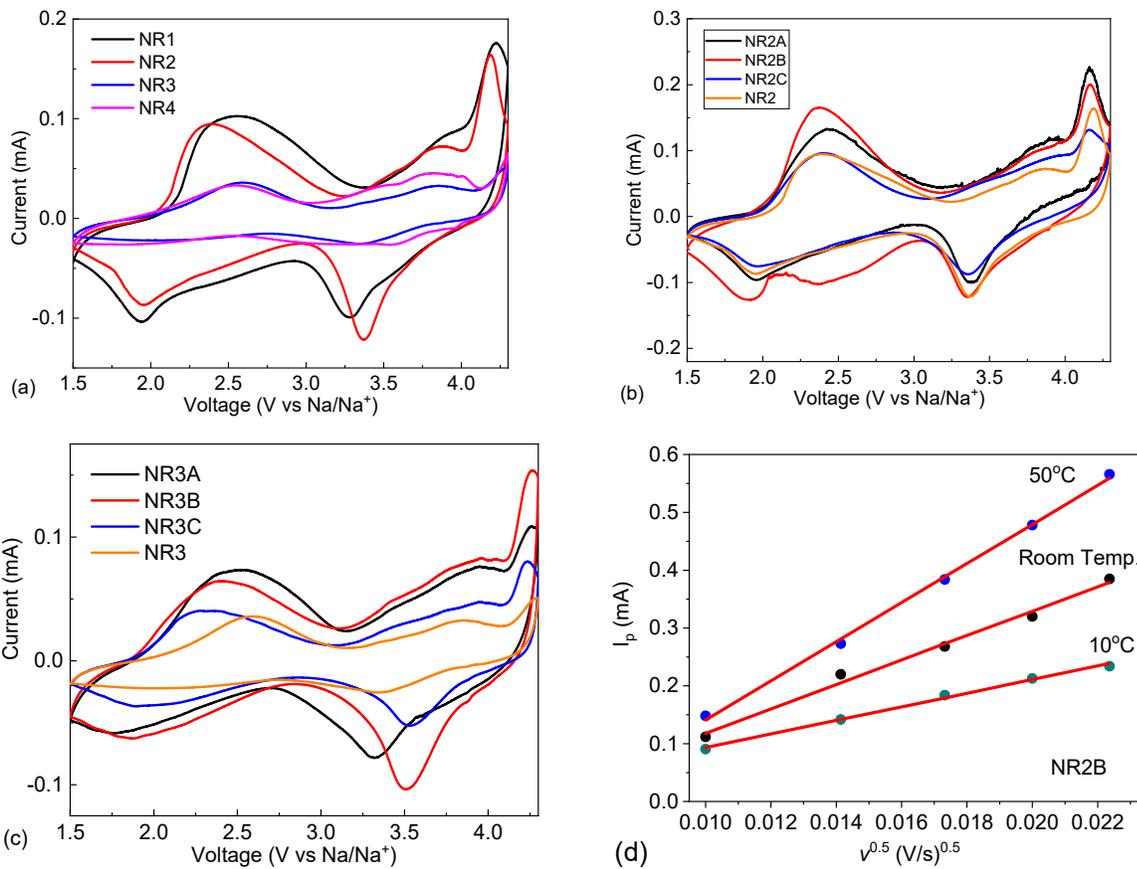


Figure S5. CV graphs of (a) NR0, NR1, NR2, NR3 and NR4, (b) NR2, NR2A, NR2B and NR2C and (c) NR3, NR3A, NR3B and NR3C

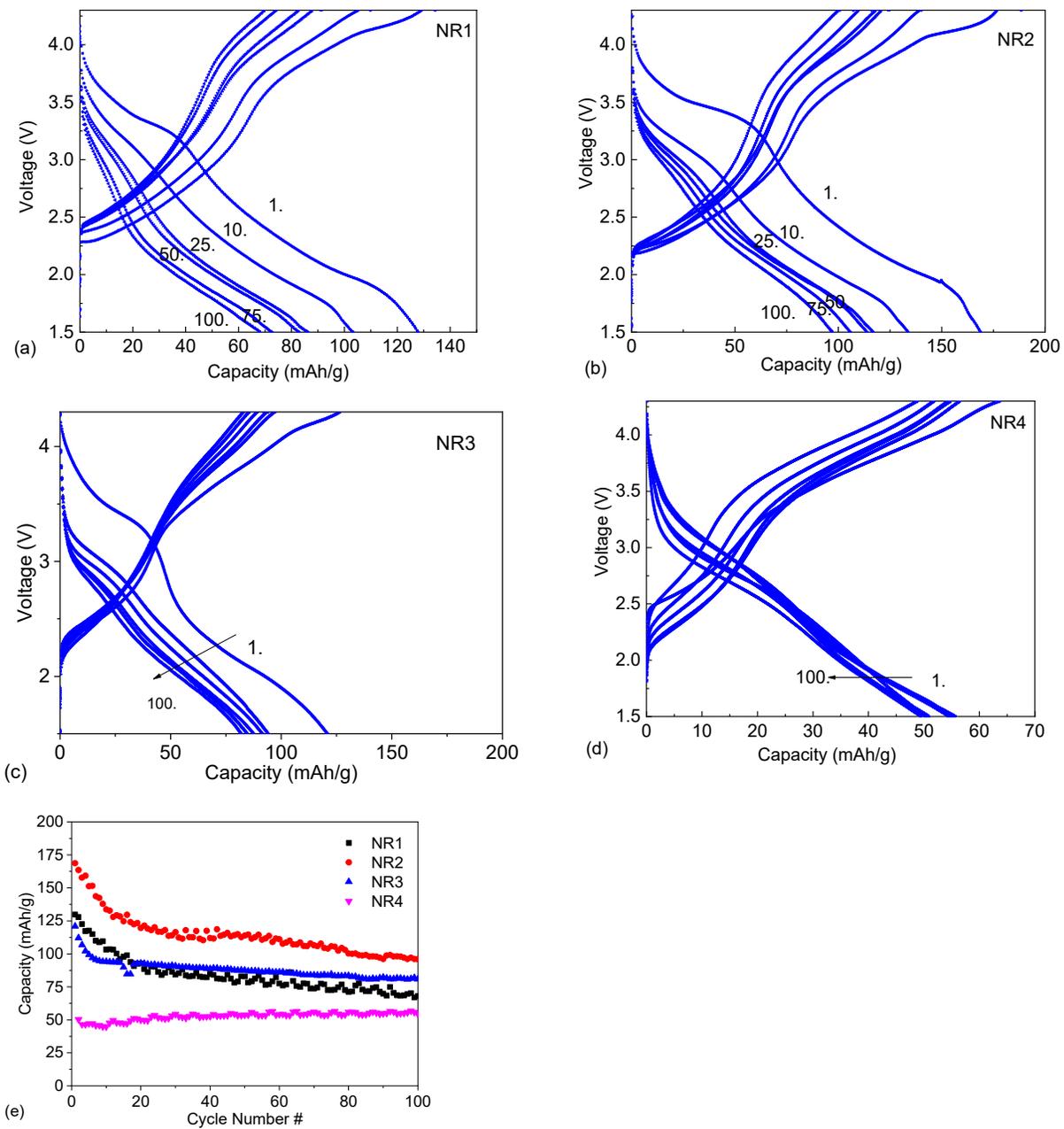


Figure S6. Charge-discharge curves for (a) NR1, (b) NR2, (c) NR3, (d) NR4 and (e) their cycling stability.

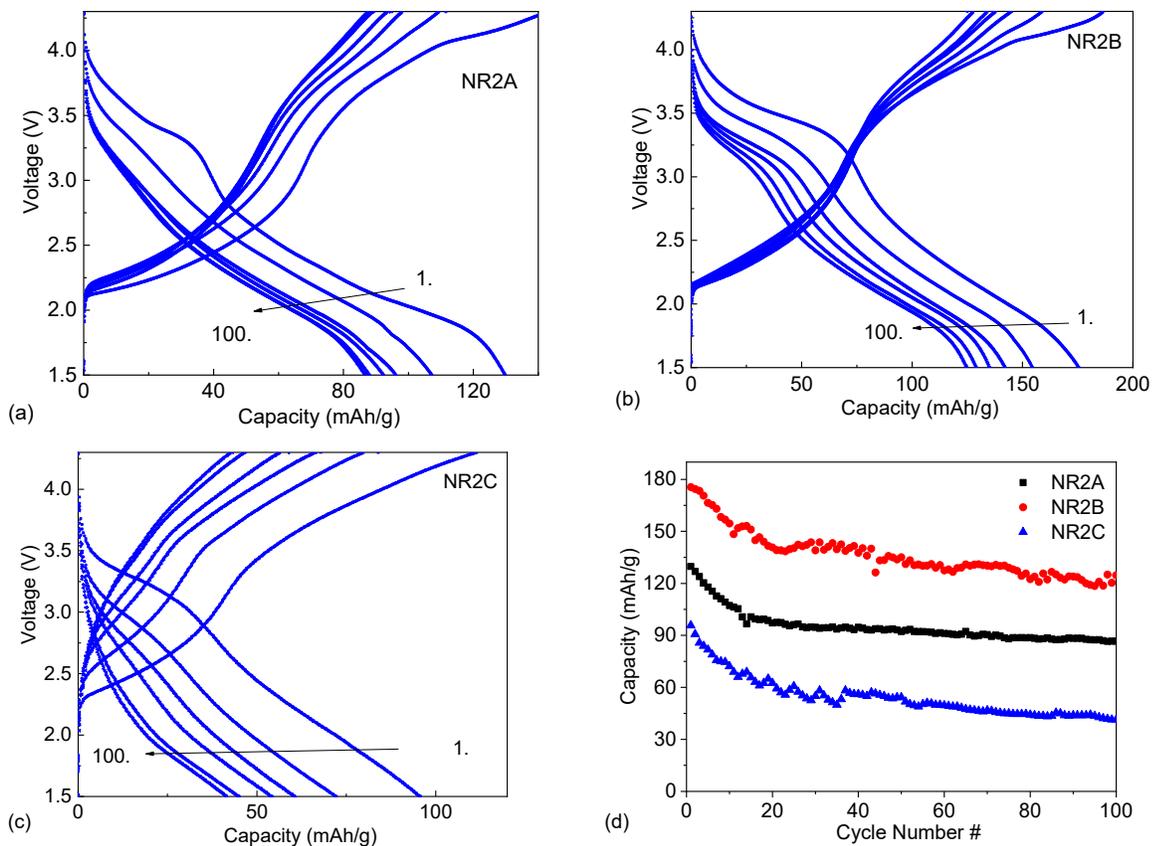
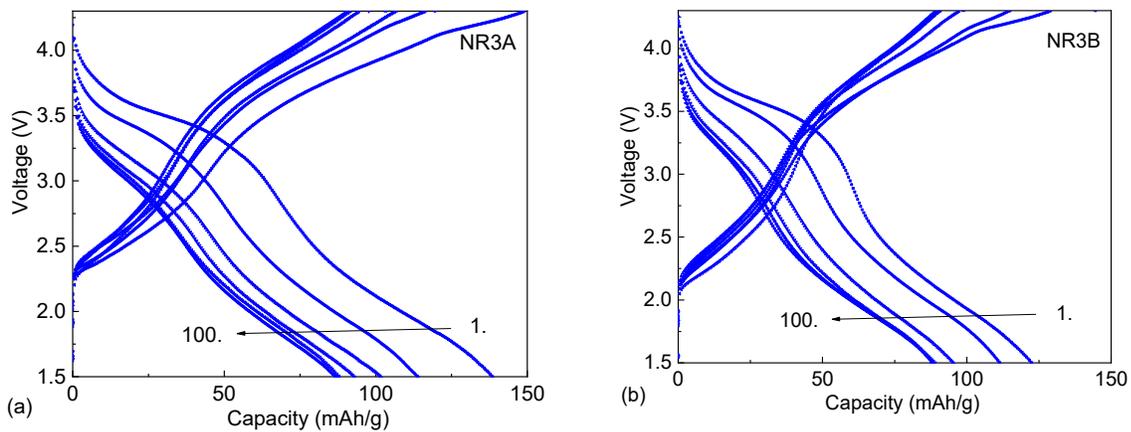


Figure S7. Charge-discharge curves for (a) NR2A, (b) NR2B, (c) NR2C, and their (d) cycling stability.



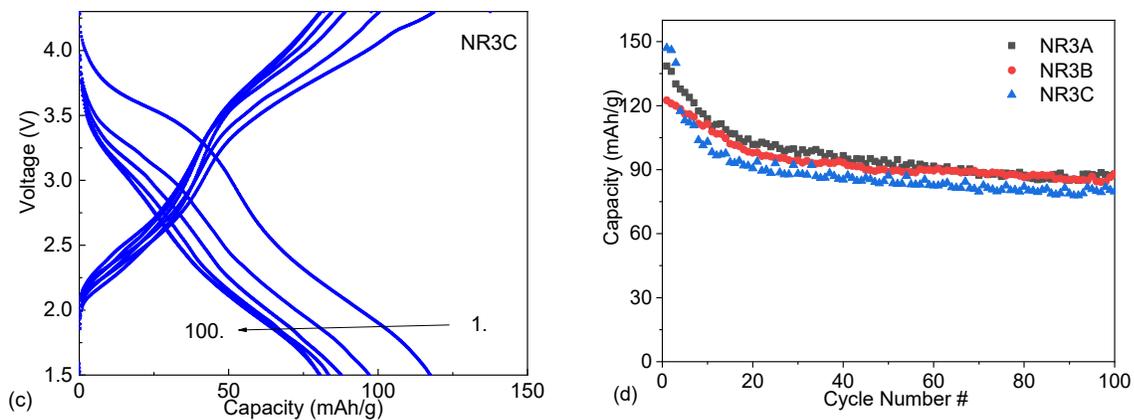
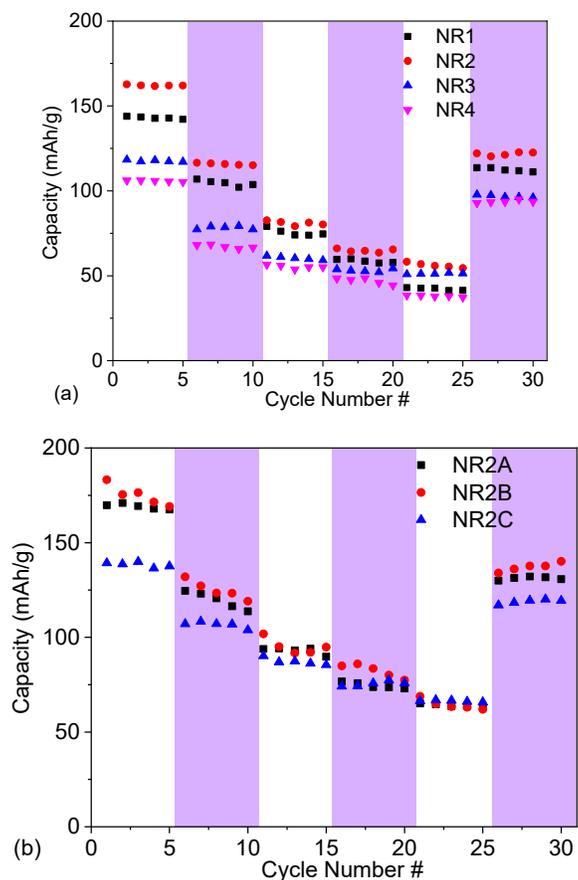


Figure S8. Charge-discharge curves for (a) NR3A, (b) NR3B, (c) NR3C, and their (d) cycling stability.



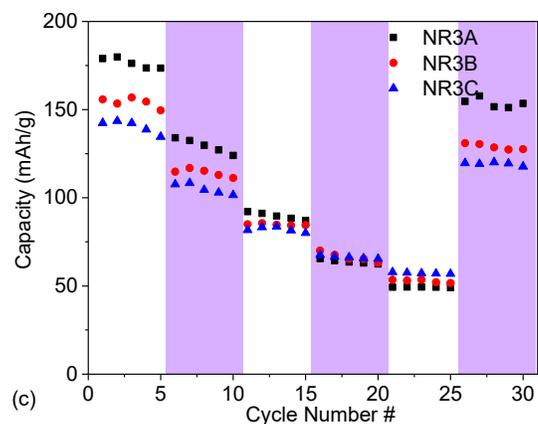


Figure S9. C-rate graphs of (a) NR0, NR1, NR2, NR3 and NR4, (b) NR2, NR2A, NR2B and NR2C and (c) NR3, NR3A, NR3B and NR3C for 10-40-80-120-150-10 mA/g current rate respectively.

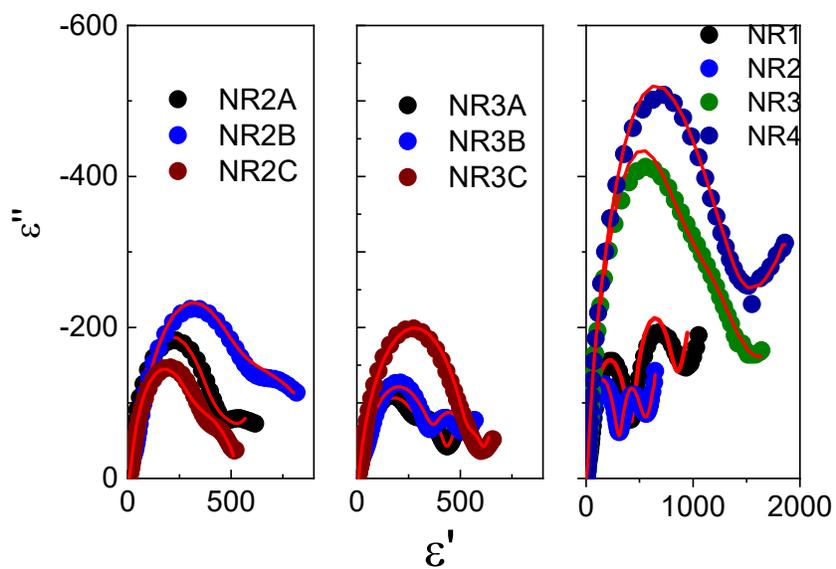


Figure S10. EIS graphs of the cells.

Table S3: EIS fitting parameters of the cells. $Q = \frac{1}{Q_y} \frac{1}{s^{Q_a}}$

| Parameters | Rs | Rc | C x 10 ⁻³ | Rq | Qy | Qs | W |
|------------|------|------|-----------------------|------|------------------------|-------|-----------------------|
| NR1 | 7.32 | 343 | 1.76 | 419 | 1.16 10 ⁻⁵ | 0.803 | 1.57 10 ⁻² |
| Nr2 | 7.85 | 1902 | 1.58 | 298 | 1.57 10 ⁻⁵ | 0.903 | 1.89 10 ⁻² |
| NR3 | 5.28 | 562 | 1.68 | 937 | 26.7 10 ⁻⁵ | 0.567 | 1.59 10 ⁻² |
| NR4 | 4.28 | 1150 | 1.47 10 ⁻³ | 1800 | 8.84 10 ⁻⁵ | 0.639 | 1.94 10 ⁻³ |
| NR2A | 5.46 | 3010 | 6.49 10 ⁻⁶ | 2350 | 0.51 10 ⁻⁵ | 0.560 | 9.451 0 ⁻³ |
| NR2B | 7.09 | 2970 | 1.52 10 ⁻⁵ | 7250 | 0.434 10 ⁻⁵ | 0.434 | 4.39 10 ⁻³ |
| NR2C | 6.49 | 2050 | 9.71 10 ⁻⁶ | 3340 | 0.498 10 ⁻⁵ | 0.527 | 5.18 10 ⁻³ |
| NR3A | 5.92 | 84 | 0.883 | 323 | 4.54 10 ⁻⁵ | 0.716 | 2.07 10 ⁻² |
| NR3B | 8.25 | 109 | 2.3 | 372 | 4.51 10 ⁻⁵ | 0.718 | 1.93 10 ⁻² |
| NR3C | 8.72 | 50.7 | 3.65 | 530 | 2.15 10 ⁻⁵ | 0.813 | 2.55 10 ⁻² |

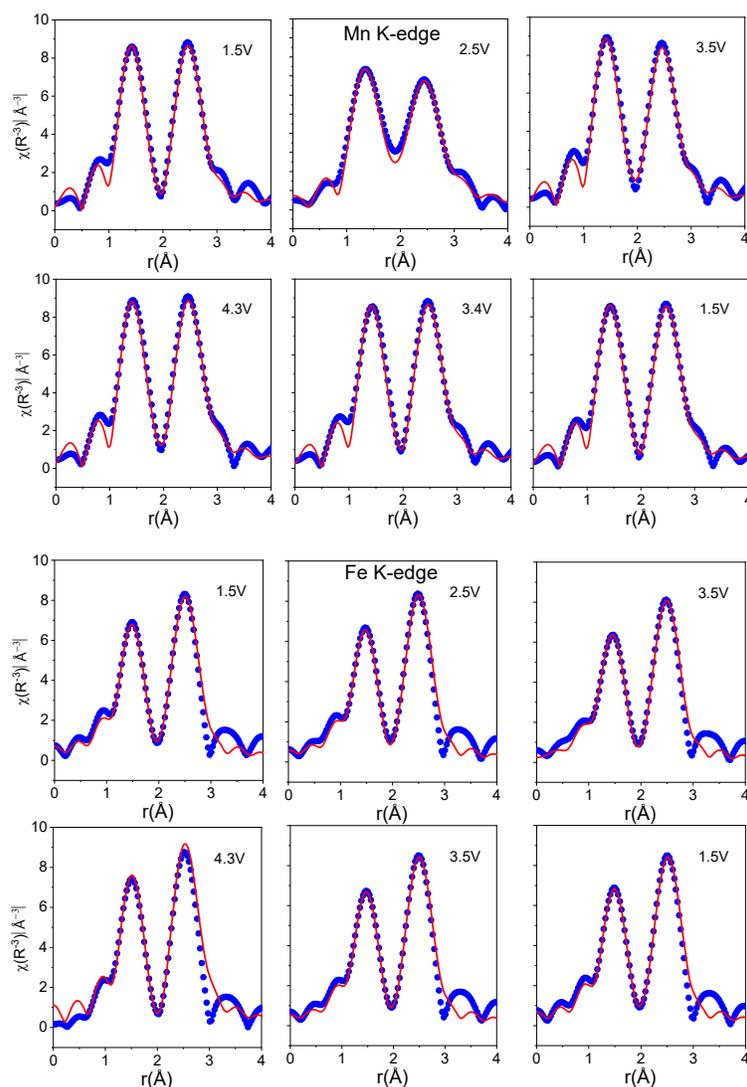


Figure S11. Artemis fitting of NR2B cells for Mn and Fe k edge for different voltage values