Supplementary Information

Suppressing H2-H3 phase transition in high Ni- low Co cathode material by dual modification

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Fig. S1. Schematic illustration of dual modification of Boron doping and BPO₄ surface coating on NCM cathode.



Fig. S2. Rietveld refinement results of (a) B-NCM (b) NCM@BP (c) 2B-NCM@2BP

Sample	Site	X	У	Z	occupancy	Ni in Li site
NCM94	Li1	0.0	0.0	0.5	0.9621	_
	Ni1	0.0	0.0	0.0	0.9021	_
	Li2	0.0	0.0	0.0	0.0379	_
	Ni2	0.0	0.0	0.5	0.0379	3.79%
	Co1	0.0	0.0	0.0	0.03	_
	Mn1	0.0	0.0	0.0	0.03	_
	01	0.0	0.0	0.2420	1.000	-
Sample	Site	X	У	Z	occupancy	Ni in Li site
B-NCM@BP	Li1	0.0	0.0	0.5	0.9742	_
	Ni1	0.0	0.0	0.0	0.9142	_
	Li2	0.0	0.0	0.0	0.0258	_
	Ni2	0.0	0.0	0.5	0.0258	2.58%
	Co1	0.0	0.0	0.0	0.03	_
	Mn1	0.0	0.0	0.0	0.03	_
	01	0.0	0.0	0.2420	1.000	

Table S1. Occupancy of atoms in NCM94 and B-NCM@BP as calculated by Rietveld refinement using GSAS software



Fig. S3 SEM images of (a) NCM94 (b) B-NCM (c) NCM@BP (d) B-NCM@BP (e) 2B-NCM@2BP

Sample	Ni	Peak position (eV)	Fraction (%)
NCM04	Ni ²⁺	854.6	50.77
NC1914	Ni ³⁺	855.56	49.23
	Ni ²⁺	854.6	12.33
B-NCM@BP	Ni ³⁺	855.6	87.67

Table S2. XPS peak fitting for Peak position and fractions of Ni for NCM94 and B-NCM@BP.

Sample	Element	Peak position (eV)	Oxidation state
	Со	779.59/794.79	+3
NCM94	Mn	642.12	+4
	0	528.55/531.08	-2
	Со	779.59/794.79	+3
	Mn	642.12	+4
B-NCM@BP	0	528.30/530.78	-2
	В	190.88	+3
	Р	133.37	+3

Table S3. XPS fitting results for peak position and oxidation state of elements for NCM94 and B-NCM@BP.



Fig. S4. Cyclic voltammetry curves of (a) NCM94 (b) B-NCM@BP for the initial 5th cycles.

Sample	No. of cycles	$R_{sf} + R_{ct}$	σ	D _{Li+} (cm ² S ⁻¹)
NCM94	3 rd	34.71	127.84	3.51×10^{-12}
	100 th	42.13	147.57	2.63×10^{-12}
B-NCM@BP	3 rd	20.5	53.56	2×10^{-11}
	100 th	23.48	75.78	1.02×10^{-11}

Table. S4 EIS fitting results and calculated D $_{Li^+}$ after 3rd and 100th cycles.



Fig. S5. In-situ XRD patterns of (a) NCM94 and (b) B-NCM@BP during first cycle



Fig. S6. SEM images of (a, c) after 3rd cycle and (b, d) after 100th cycles of NCM94 and B-NCM@BP respectively.