Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

The effects of Ni ions' charge disproportionation on the high electrochemical performance of $Ni_{1-x}Co_xO$ nanoparticles

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Experiment section

Materials characterization

The compositions of samples were investigated using energy-dispersive X-ray spectroscopy (EDS) attached to a scanning electron microscope (MAagellan-400).

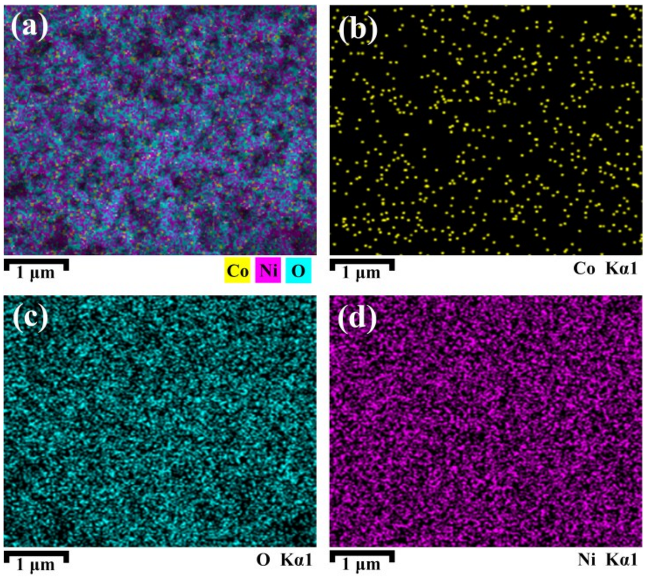

Figure S1. Elemental mapping images of $Ni_{1-x}Co_xO$ (x=0.055) nanoparticles. (a) The electronic image of total elements; (b) Co Kα1; (c) O Kα1 and (d) Ni Kα1.

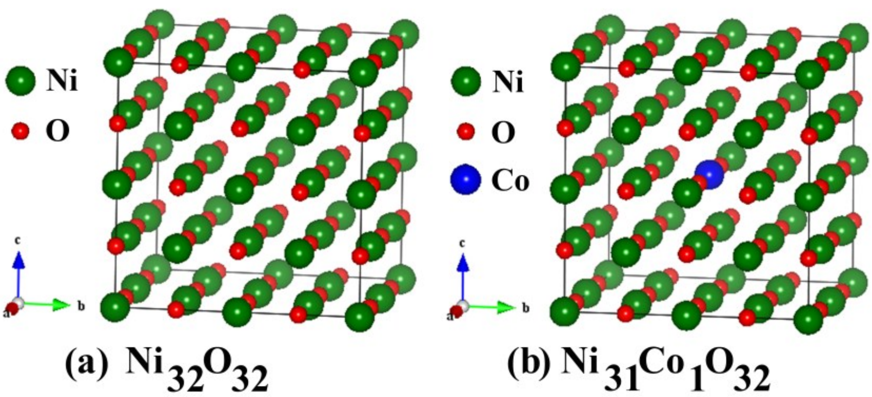

Figure S2. The models of (a) $Ni_{32}O_{32}$, (b) $Ni_{31}Co_1O_{32}$ respectively.

Table S1. The integral intensity of PDOS for each band of Ni-3d orbital and O-2p orbital energy levels.

		e_g*	e_g^b	T_{2g}	Total
Ni-3d	$Ni_{32}O_{32}$	52.3135	111.1668	101.5453	265.0256
	$Ni_{31}Co_1O_{32}$	52.8885	110.8735	101.3808	265.1428
O-2p	$Ni_{32}O_{32}$	14.7985	7.3345	7.9502	30.0832
	$Ni_{31}Co_1O_{32}$	14.7592	7.2093	7.9074	29.8759

Table. S2. The effective mass of the energy band near the Fermi energy level corresponding to the $Ni_{32}O_{32}$ and $Ni_{31}Co_1O_{32}$ structures.

Structures	Fermi level (eV)	Electron effective mass	m_0 (Kg)
$Ni_{32}O_{32}$	0	0.0057 m_0	9.10938215(45)× 10^{-31}
$Ni_{31}Co_1O_{32}$	0	0.0096 m_0	9.10938215(45)× 10^{-31}

The electron effective mass values of $Ni_{31}Co_1O_{32}$ structure are higher than that of $Ni_{32}O_{32}$ structure, which indicates that the conductive ability of $Ni_{31}Co_1O_{32}$ structure are higher than that of $Ni_{32}O_{32}$ structure. Therefore, the $Ni_{1-x}Co_xO$ electrode materials with good electrical conductivity exhibits the better electrochemical performance.

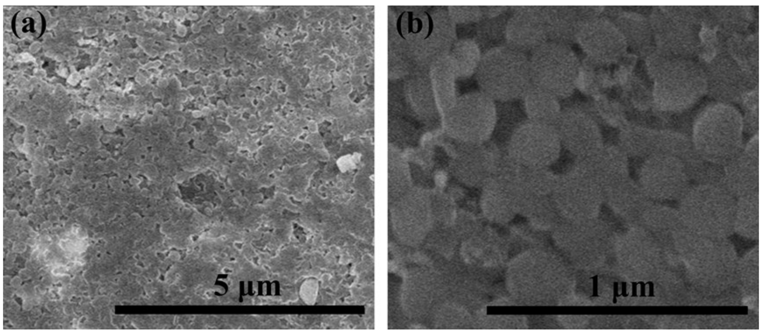

Fig. S3. (a) Low magnifification and (b) high magnifification FESEM image of $Ni_{1-x}Co_xO$ (x=0.055) electrode before 50,000 GCD cycles.

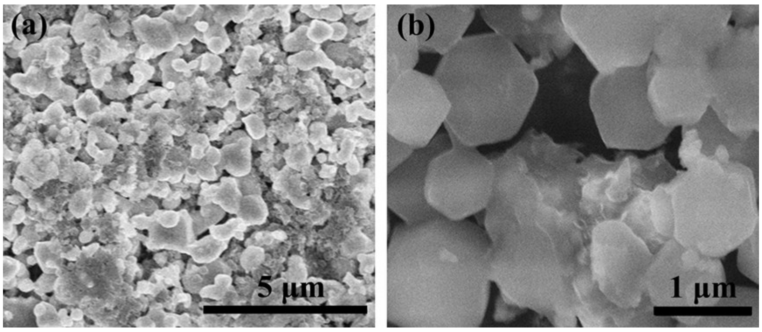

Fig. S4. (a) Low magnifification and (b) high magnifification FESEM image of $Ni_{1-x}Co_xO$ (x=0.055) electrode after 50,000 GCD cycles.

Table S3. Comparison of the specific capacitance of $Ni_{1-x}Co_xO$ electrodes with some recently reported materials.

Materials/ electrodes	Current density	Electrolyte	Specific capacitance	Reference
NiCoO-net	1.5 A g^{-1}	2 M KOH	1060.0 F g-1	[1]
Ni-Co-O-1	1 A g^{-1}	6 M KOH	722.0 F g^{-1}	[2]
Ni-Co oxide	1 A g^{-1}	6 M KOH	1539.0 F g^{-1}	[3]
Co-doped NiO	6 A g^{-1}	1 M KOH	720.0 F g^{-1}	[4]
NCOs	1 A g^{-1}	1 M KOH	506.0 F g^{-1}	[5]
Mn-NiO	5 mA cm^{-2}	6 M KOH	1166.0 F g^{-1}	[6]
$NiCo_2O_4$@NiO	2 A g^{-1}	1 M KOH	1188.0 F g^{-1}	[7]
$Ni_{1-x}Co_xO$ (x=0.055)	1 A g^{-1}	6 M KOH	**1665.3 F g^{-1}**	this work

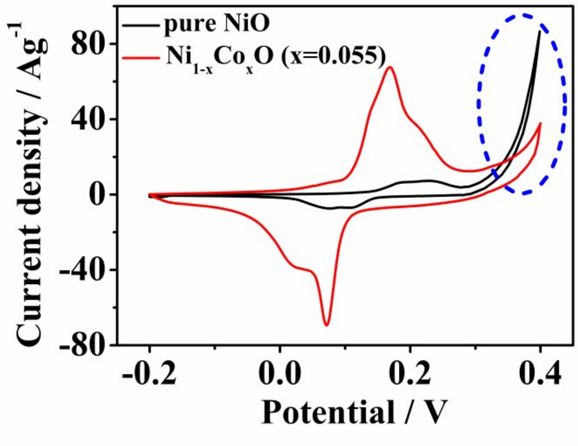

Fig. S5. CV curves of NiO and $Ni_{1-x}Co_xO$ (x=0.055) electrode materials at a sweep rate of 1 mV s^{-1}.

Reference

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