

## Supporting information

# An effective lithium incorporation strategy to boost the charge-storage capacity of bimetallic metal-organic frameworks with theoretical insights and solid-state lithium-ion capacitors

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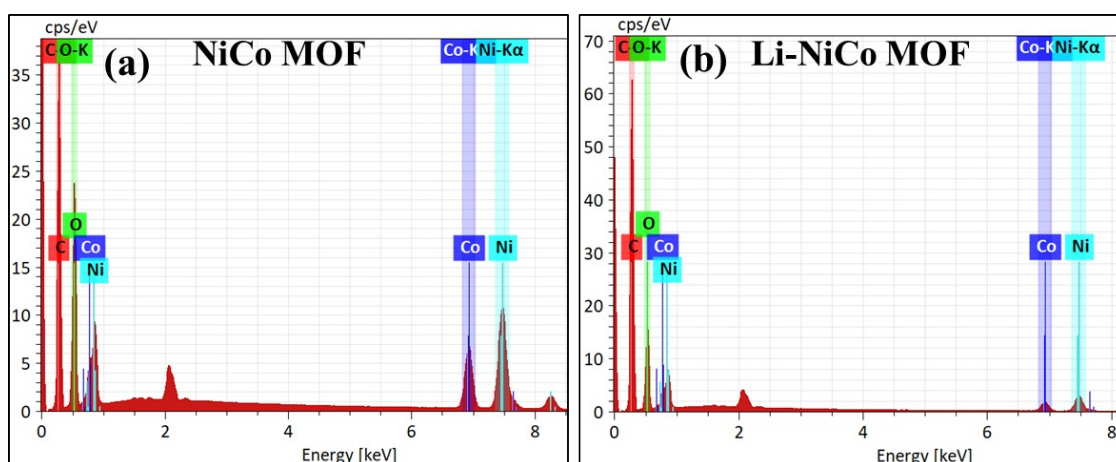


Fig. S1. Depict the EDS elemental composition of (a) NiCo MOF and (b) Li-NiCo MOF.

NiCo MOF				Li-NiCo MOF			
Element	At. No.	Mass Norm. [%]	Atom [%]	Element	At. No.	Mass Norm. [%]	Atom [%]
C	6	43.96	61.99	C	6	60.22	70.62
O	8	28.38	30.04	O	8	30.98	27.27
Co	27	9.48	2.72	Co	27	2.87	0.69
Ni	28	18.17	5.24	Ni	28	5.93	1.42
		<b>100.00</b>	<b>100.00</b>			<b>100.00</b>	<b>100.00</b>

Fig. S2. Concentration percentage of the elements in NiCo MOF and Li-NiCo MOF.

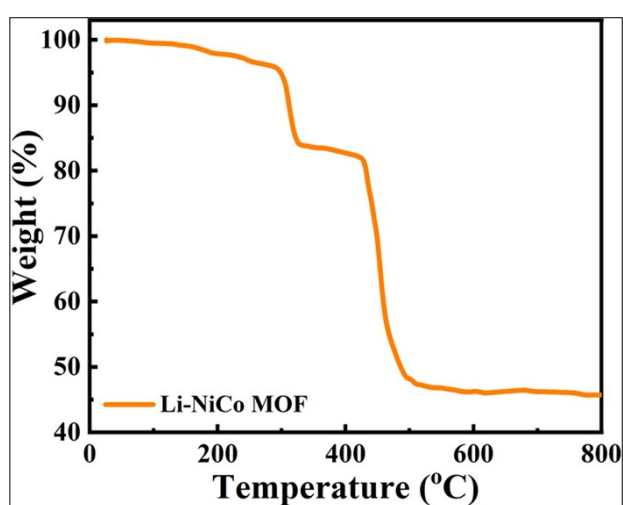


Fig. S3. TGA curve of Li-NiCo MOF.

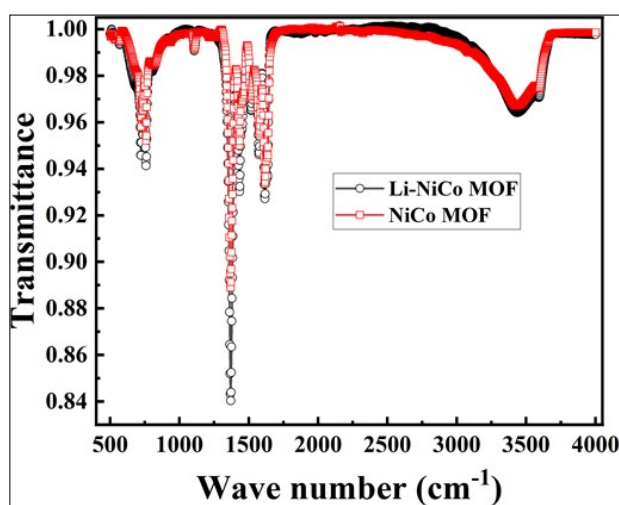


Fig. S4. Normalized FTIR plot for NiCo MOF and Li-NiCo MOF.

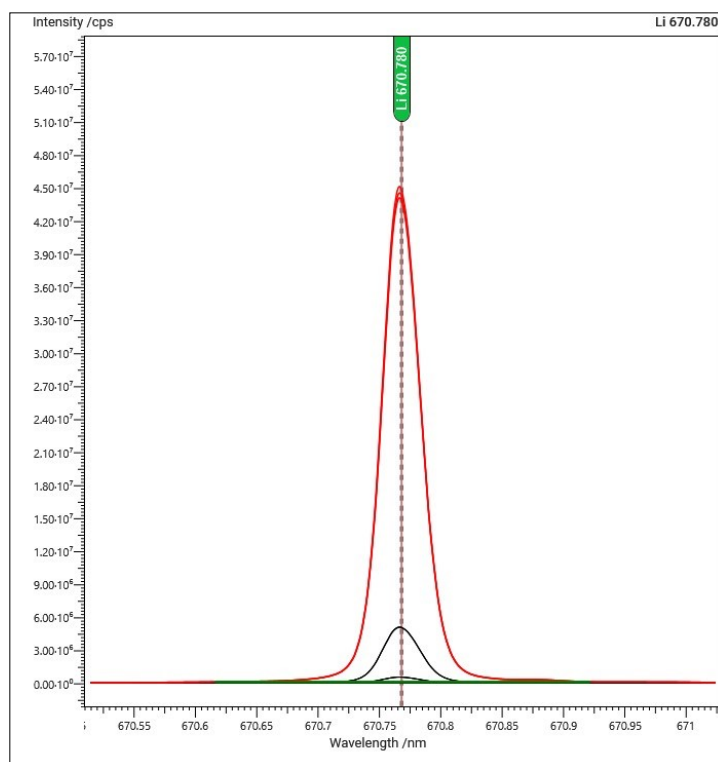


Fig. S5. ICP-OES data depicts the Li peak in Li-NiCo MOF

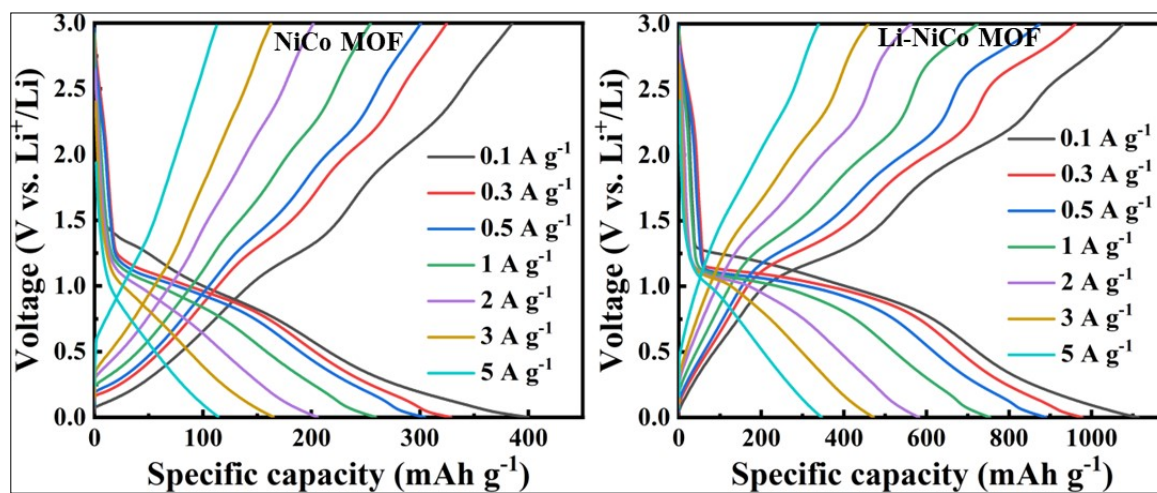


Fig. S6. CV profile for NiCo MOF and Li-NiCo MOF at different current density 0.1 to 5 A  $g^{-1}$ .

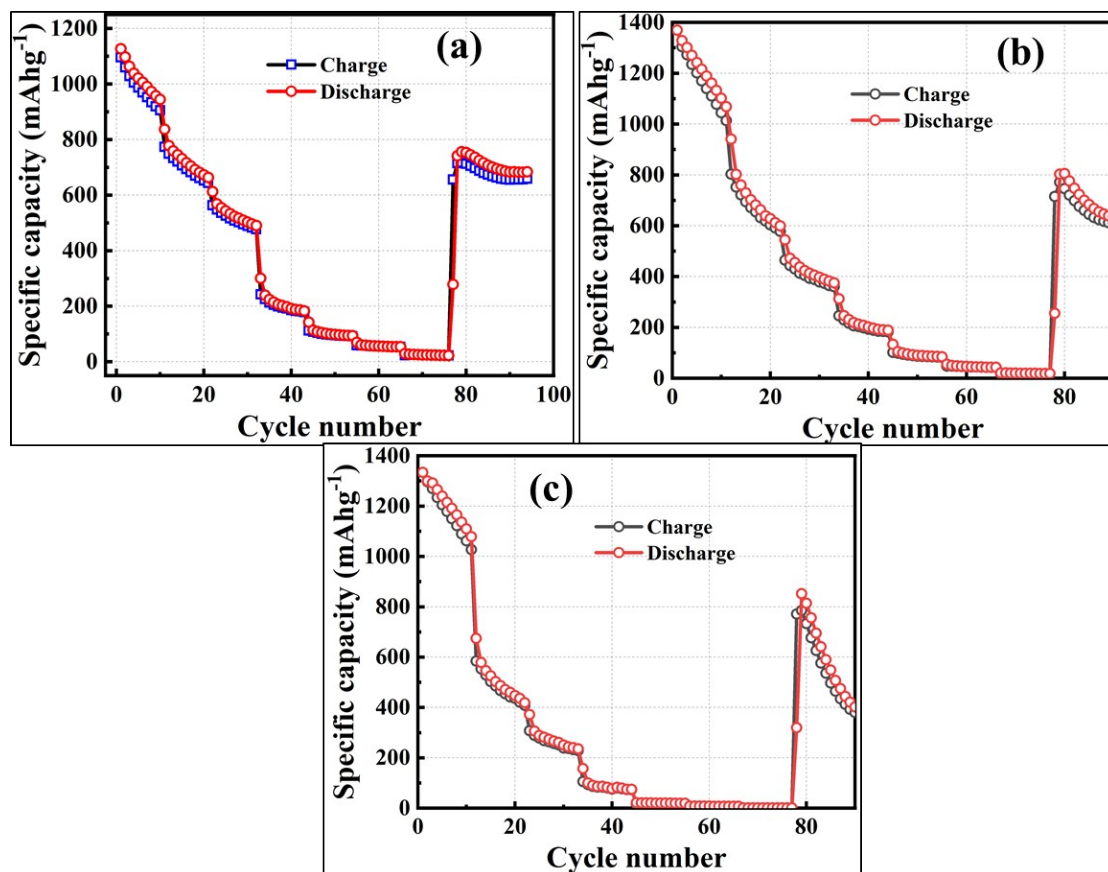


Fig. S7. Rate capability behavior for high Li-incorporated NiCo MOF prepared using (a) 2, (b) 3, and (c) 4 mmol of LiNO<sub>3</sub>.

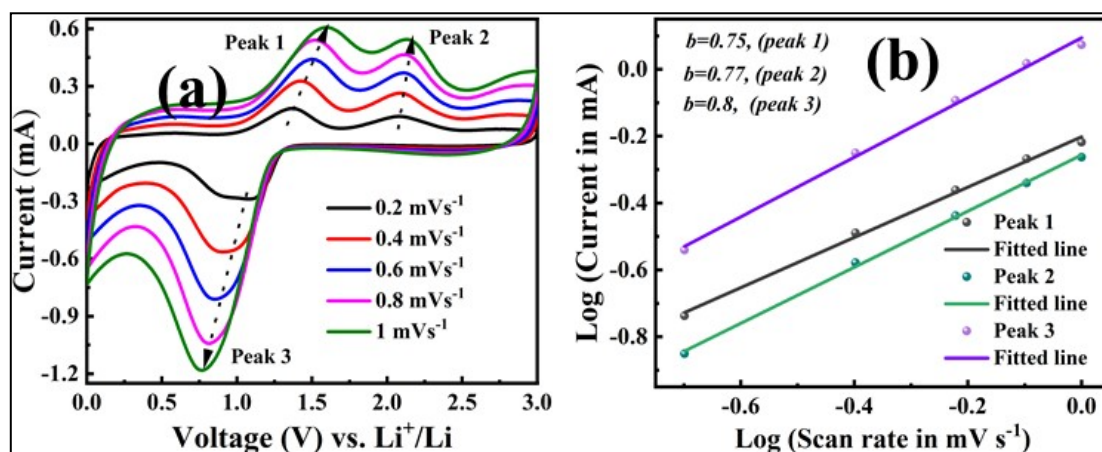


Fig. S8. (a) CV curves at different scan rates, and (b) b-value calculation by plotting log (scan rate) vs. log (current), for NiCo MOF.

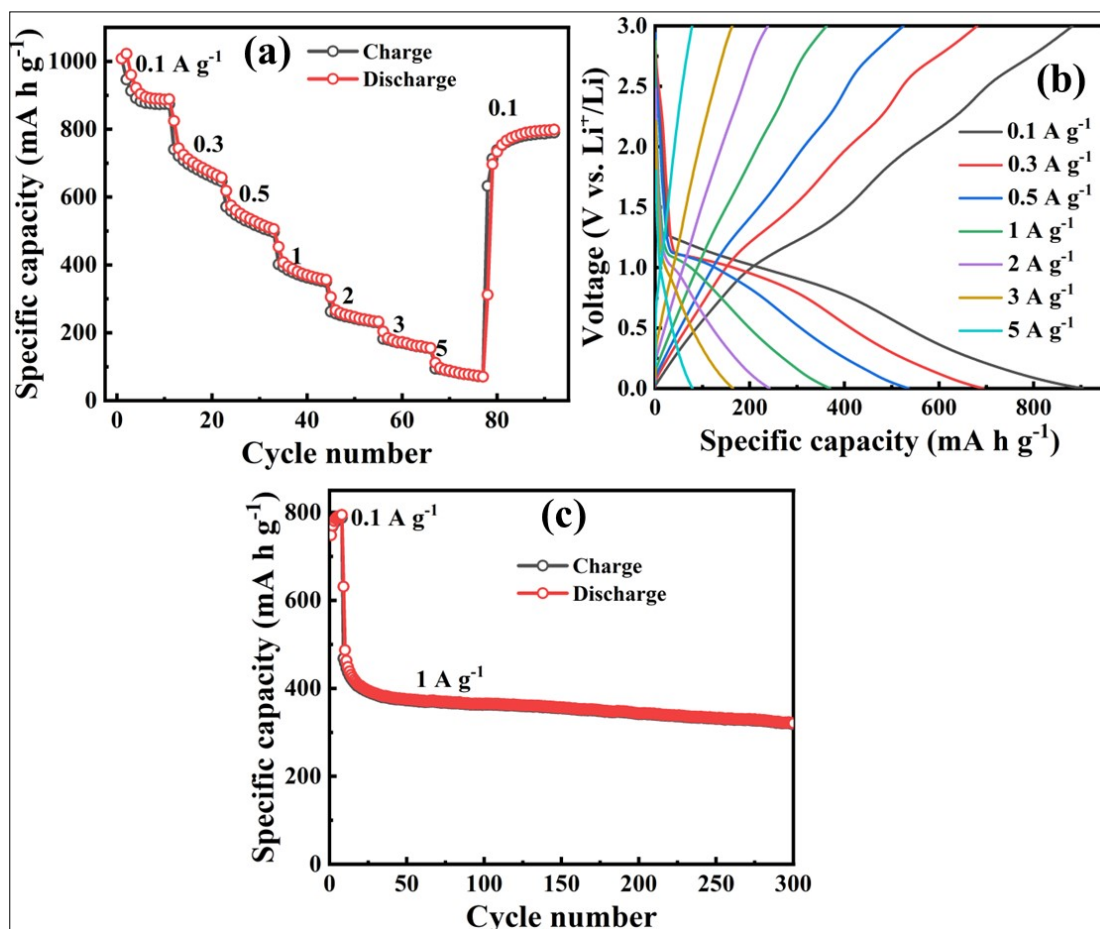


Fig. S9. (a) rate capability, (b) CD profile at different current densities, and (f) cycling capacity for 300 cycles Li-NiCo MOF prepared by sonochemical method.



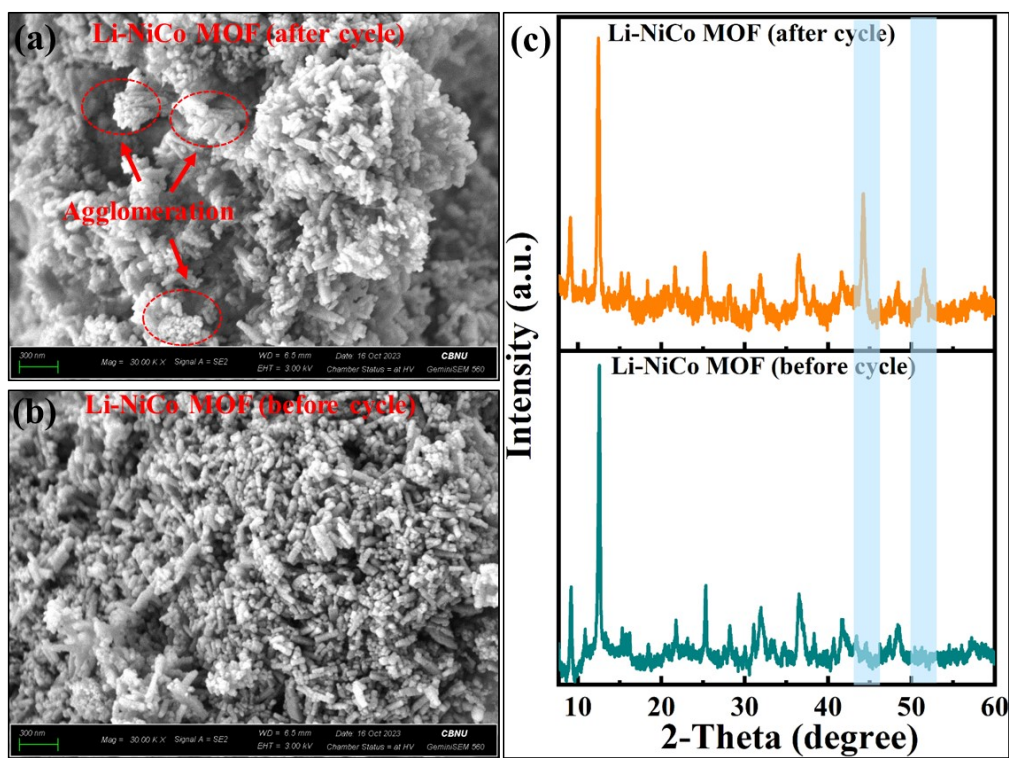


Fig. S10. SEM image of Li-NiCo MOF (a) after and (b) before the cycle test, and (c) XRD spectra for Li-NiCo MOF, before and after the cycle test.

## CONTCAR file of NiCo MOF

C Co H O Ni

1.0000000000000000

0.0000000000000000 13.1517099999999996 13.1517099999999996

13.1517099999999996 0.0000000000000000 13.1517099999999996

13.1517099999999996 13.1517099999999996 0.0000000000000000

C Co H O Ni

72 6 24 48 6

Selective dynamics

Direct

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