Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.
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Supporting Information

Three-Dimensional Ordered Mesoporous Cobalt Nitride for Fast-kinetics and Stable-cycling Lithium Storage

1. Supplementary Figures

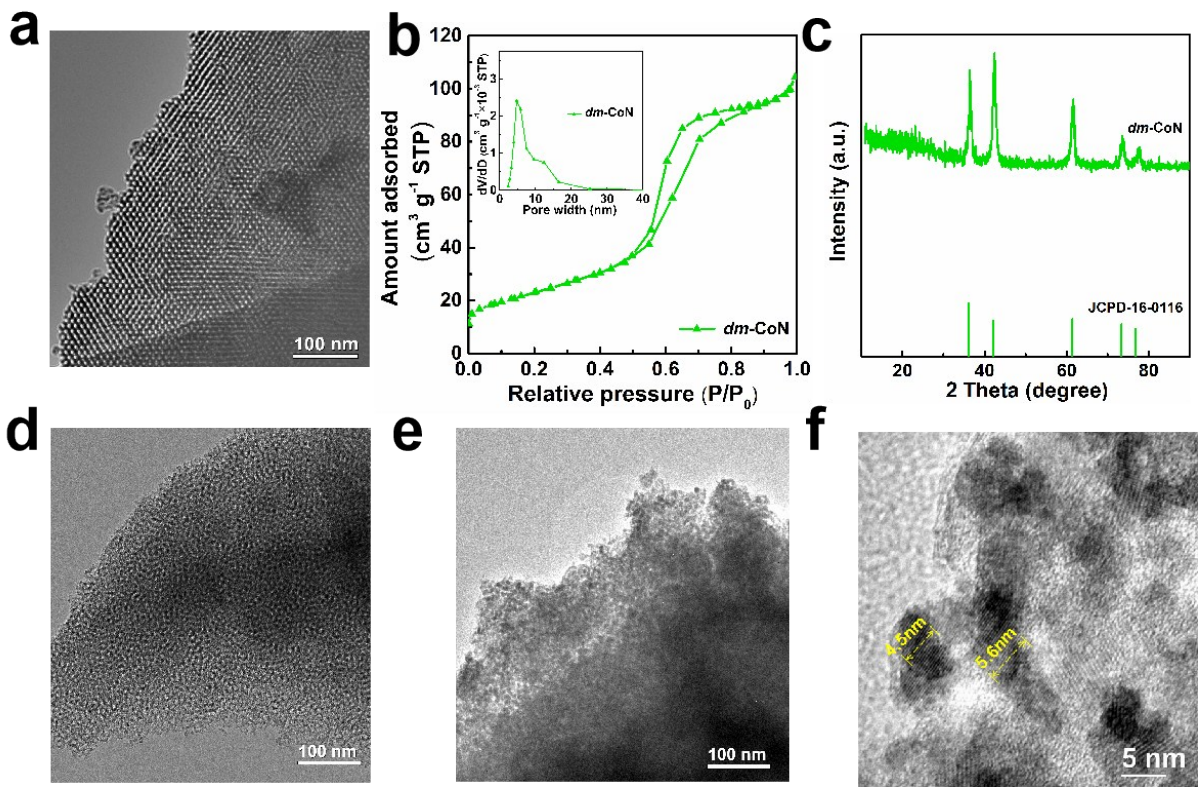

Fig. S1. a) TEM image of KIT-6 template; b) pore size distribution of *om*-CoN and *dm*-CoN; c) wide-angle XRD patterns of *dm*-CoN; d), e) TEM images of disordered SiO_2 and *dm*-CoN; f) HRTEM image of *dm*-CoN.

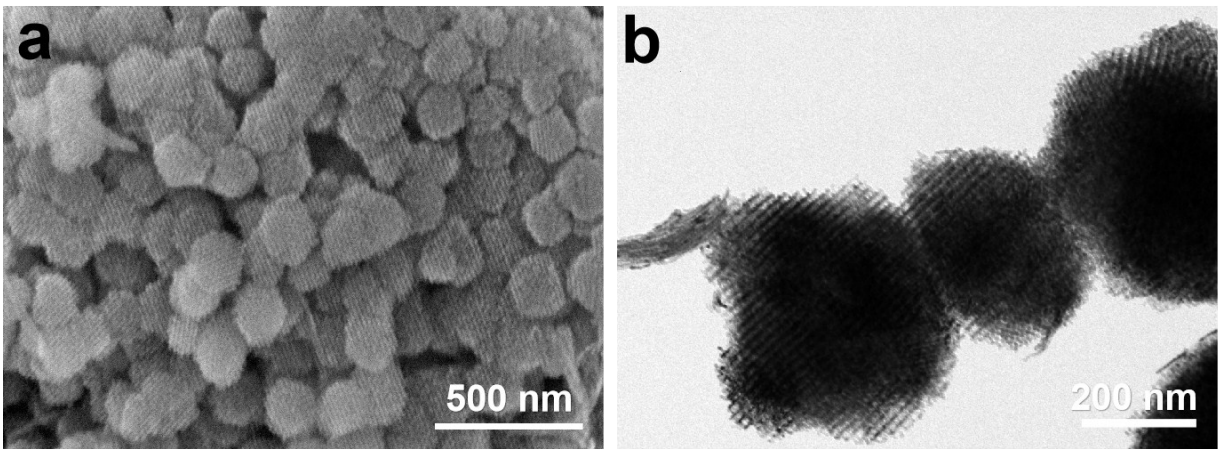

Fig. S2. a), b) Enlarged SEM and TEM images of *om*-CoN.

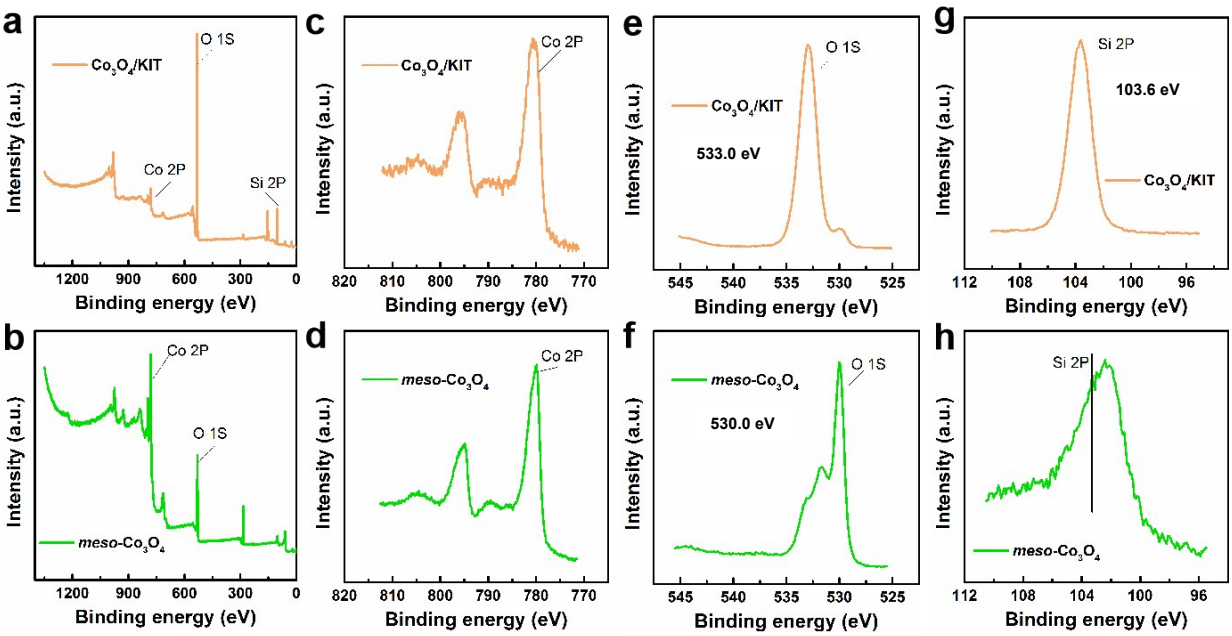

Fig. S3. a), b) The integrated XPS spectra of Co_3O_4/KIT-6 and *meso*-Co_3O_4; and the corresponding high-resolution XPS spectra of c), d) Co; e), f) O; g), h) Si.

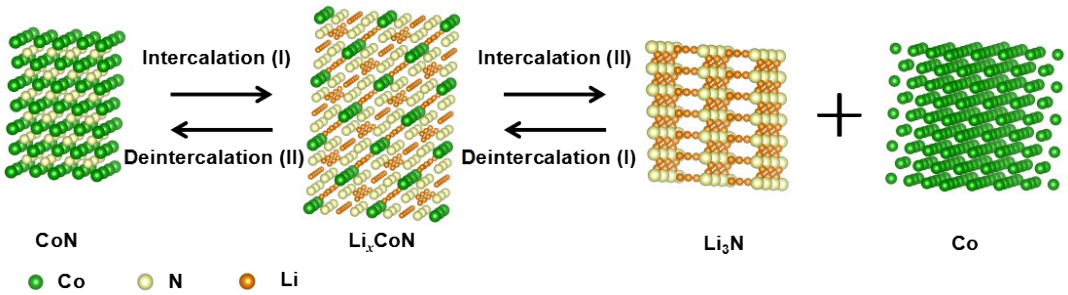

Fig. S4. Li^+ insertion/extraction-conversion mechanism in CoN.

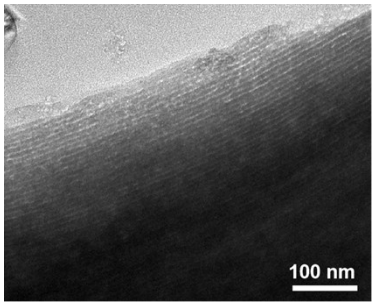

Fig. S5. TEM image of *om*-CoN after cycling.

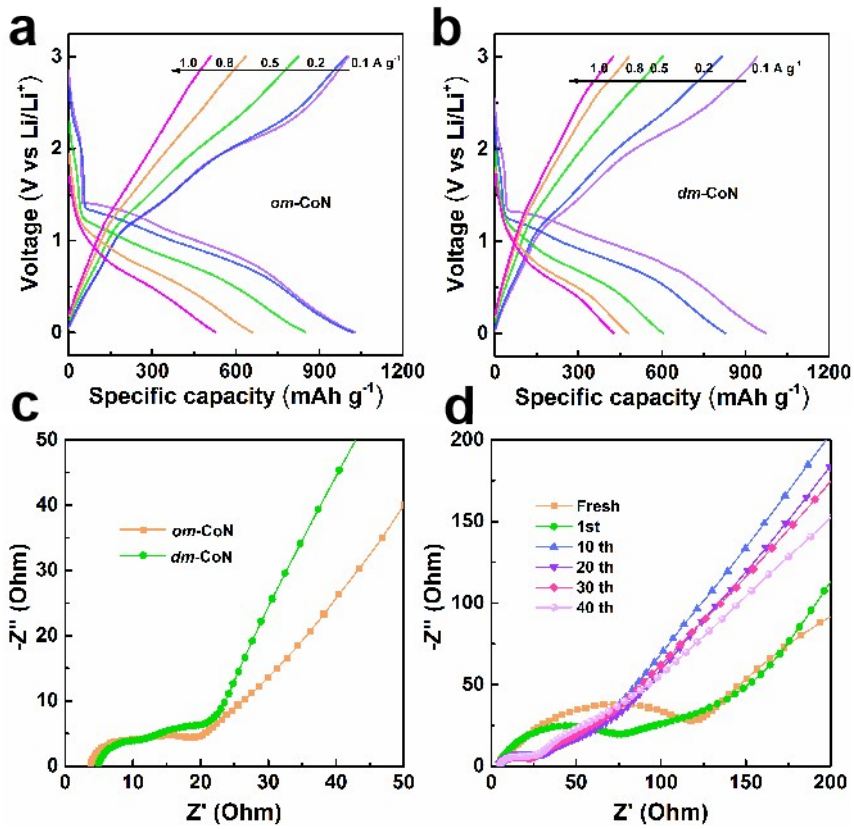

Fig. S6. a), b) Galvanostatic charge/discharge profiles at various rate for *om*-CoN and *dm*-CoN, respectively; c) EIS of *om*-CoN and *dm*-CoN after 350 cycles; d) EIS of *om*-CoN from fresh batteries to 40th cycles.

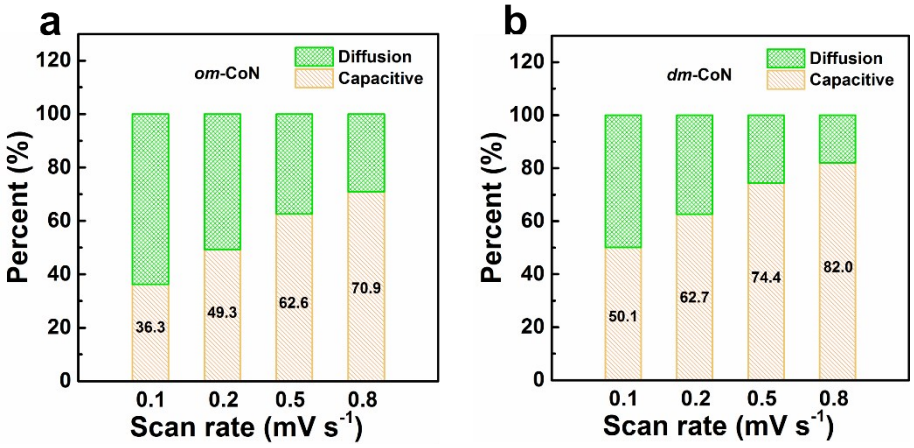

Fig. S7. a), b) Diffusion contribution in CoN at different scan rates.

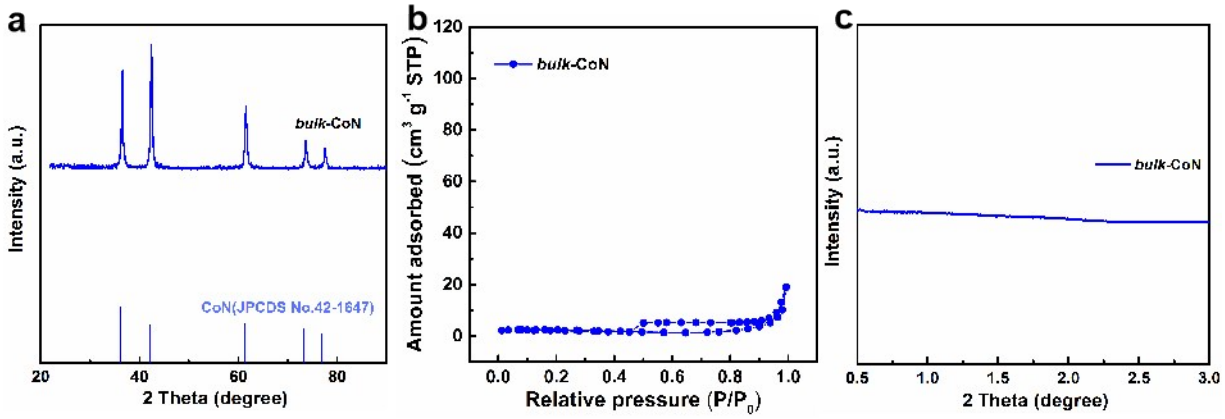

Fig. S8. a) Wide-angle XRD pattern of *bulk*-CoN; b) N_2 adsorption-desorption isotherms of *bulk*-CoN; c) small-angle XRD pattern of *bulk*-CoN.

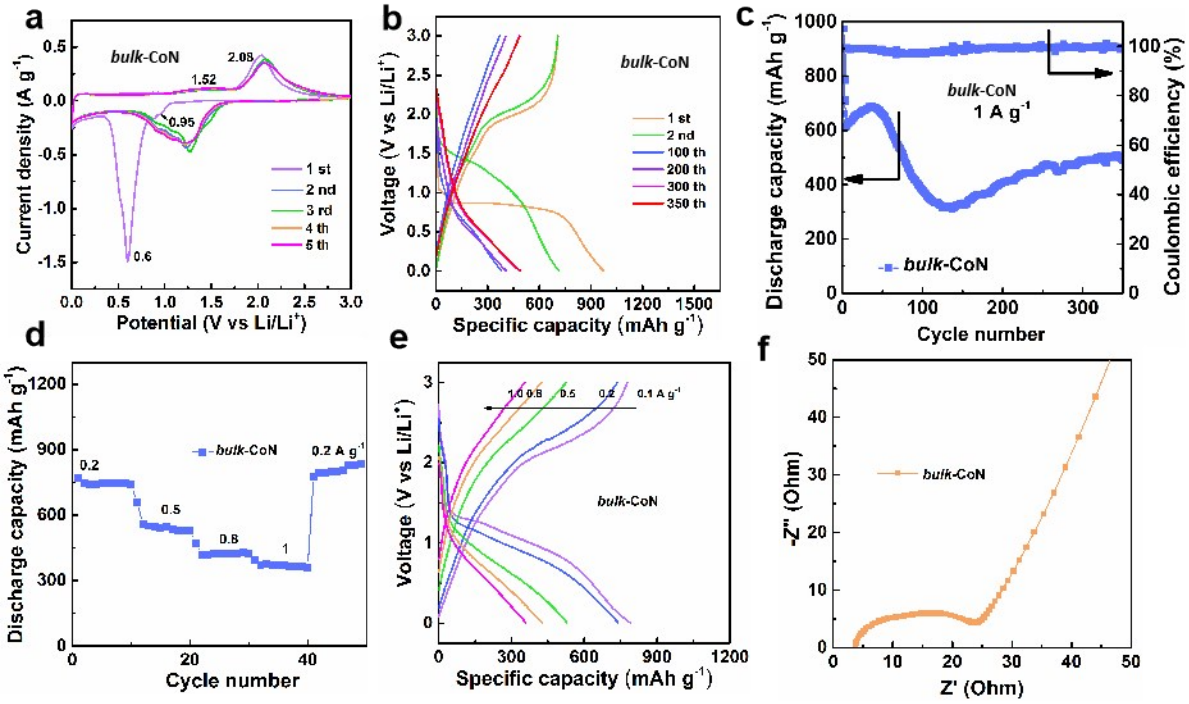

Fig. S9. a) CV curves of *bulk*-CoN electrode at 0.1 mV s^{-1}; b) galvanostatic charge/discharge profiles of *bulk*-CoN at 1 A g^{-1}; c) galvanostatic cycling performance at 1 A g^{-1} for *bulk*-CoN; d) rate performance of *bulk*-CoN; e) galvanostatic charge/discharge profiles at various rate for *bulk*-CoN; f) EIS of *bulk*-CoN.

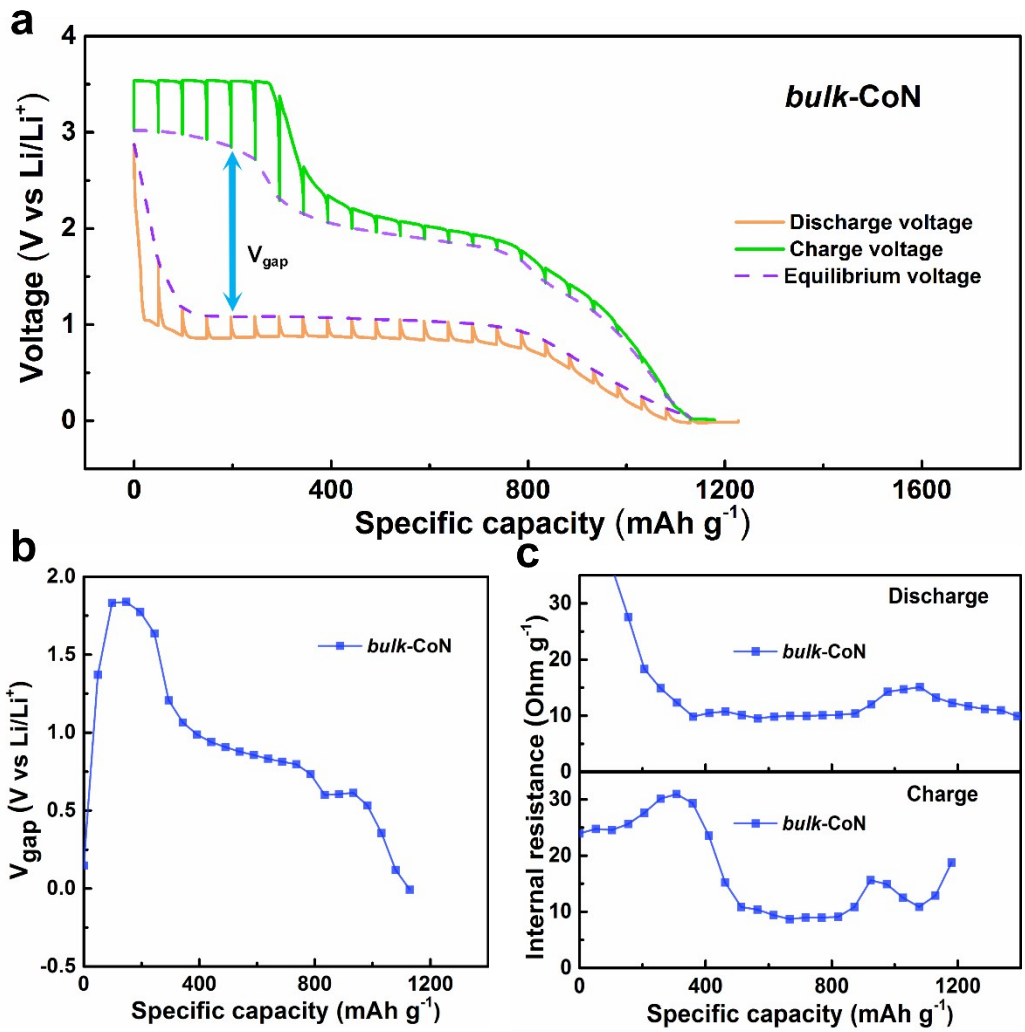

Fig. S10. a) GITT profiles of *bulk*-CoN electrodes with relaxing for 3 h after 1 h discharge/charge at 50 mA g^{-1}; b) voltage gap (V_{gap}) between charge and discharge steps after the 3 h relaxation for *bulk*-CoN; c) the internal resistance of *bulk*-CoN during discharge/charge courses.

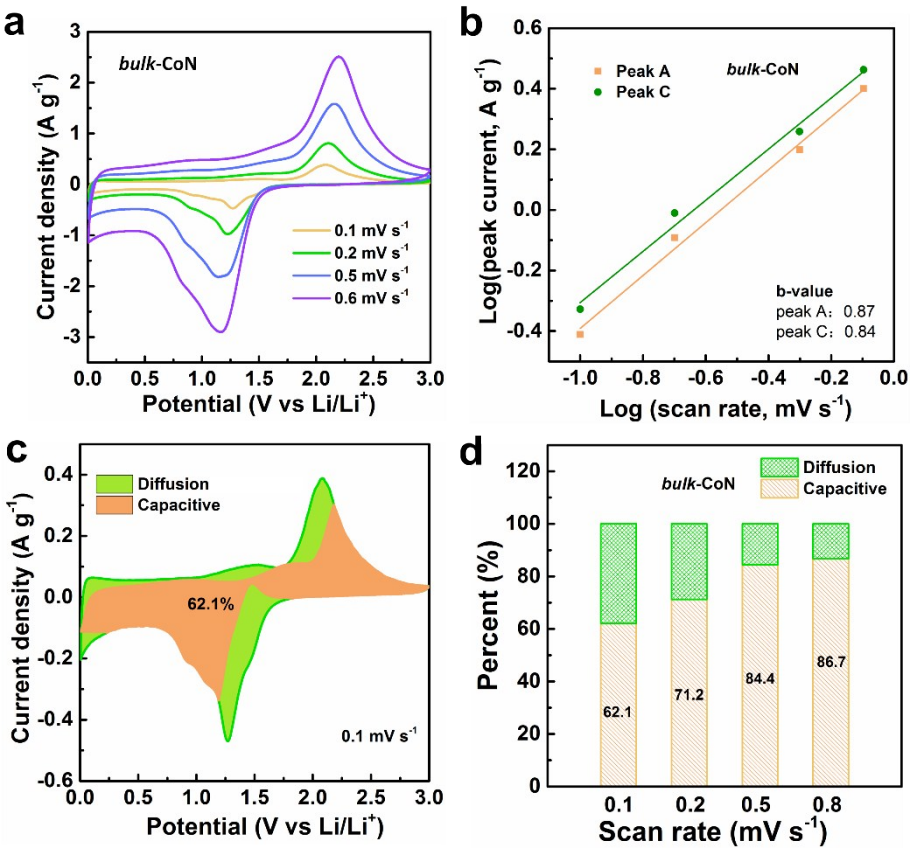

Fig. S11. a) CV curves at various scan rates from 0.1 to 0.8 mV s^{-1} for *bulk*-CoN electrode; b) logarithm peak current versus logarithm scan rate plots for *bulk*-CoN (inset: a summary of the calculated b values); c) capacitive contribution at scan rate of 0.1 mV s^{-1} in *bulk*-CoN; e) diffusion contribution in *bulk*-CoN at different scan rates.

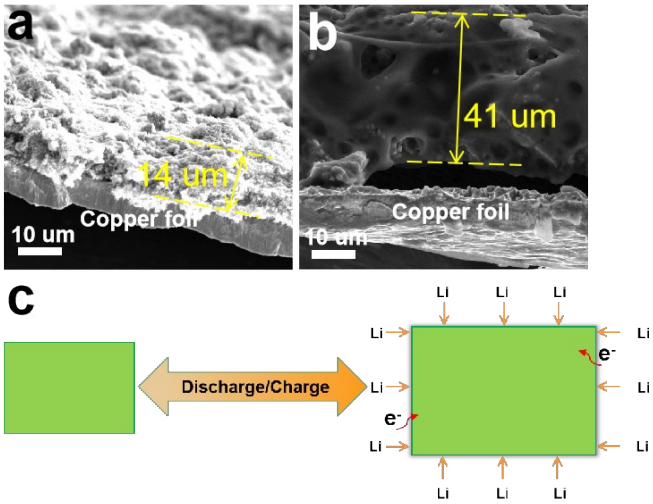

Fig. S12. Cross-sectional SEM images of *bulk*-CoN electrode: a) pristine electrode and b) fully lithiation state; c) schematic illustration for the electrochemical reactions involved in *bulk*-CoN electrode.

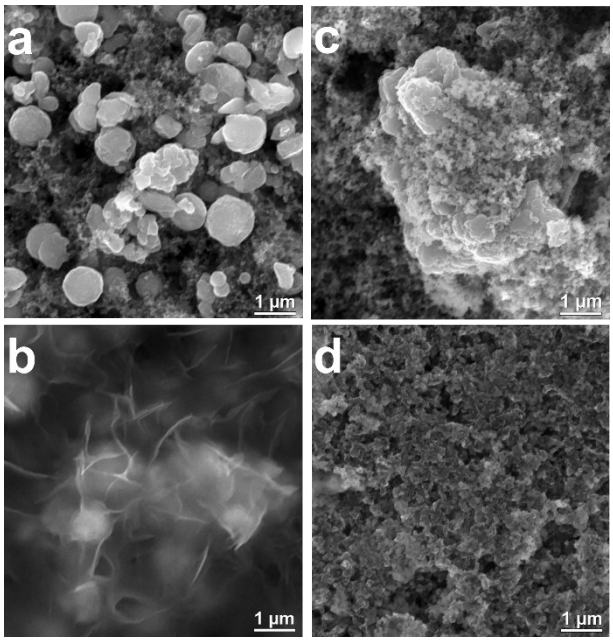

Fig. S13. SEM images of *om*-CoN a), b) and *bulk*-CoN c), d) electrodes before and after 350 cycles, respectively.

2. Supplementary Equations

$$CoN + xLi^{+} + xe^{-} \rightleftharpoons Li_xCoN; \qquad (1)$$

$$Li_xCoN + (3 - x)\ Li^{+} + (3 - x)e^{-} \longrightarrow Co^{0} + Li_3N \qquad (2)$$

Equation S1, S2. Li^{+}-intercalation/deintercalation equations.

3. Supplementary Tables

Table S1. Comparison of structural parameters of cobalt nitride in this work with previous reported works.

Nitride	BET surface area (m^2 g^{-1})	Pore size (nm)	Pore volume (cm^3 g^{-1})	Ref.
CoN	37	11.5	0.077	[1]
CoN	28	-	-	[2]
CoN	91	7.5	0.17	This work

Table S2. Structural parameters of mesostructured products and *bulk*-CoN

Sample	BET surface area（m^2 g^{-1}）	Pore volume（cm^3 g^{-1}）	Pore size（D: nm）	Cell parameter（a_0: nm）	Wall thickness（h_w: nm）
KIT-6	987	1.14	5.2	22.06	5.8
om-CoN	91	0.17	7.5	23.86	5.4
dm-CoN	83	0.16	7.7	-	-
bulk-CoN	8	0.027	-	-	-

Note: BET surface area is the specific surface area deduced from the isotherm analysis in the relative pressure range of 0.05-0.2; pore volume and pore size are calculated using the BJH method; XRD unit-cell parameter a_0 is equal to $6^{1/2}d_{211}$; the wall thickness $h_w = a_0/2 - D$.

Table S3. Performance comparison with Co-based nitrides, oxides and sulfides.

Materials	Mass loading（mg cm^{-2}）	Current density（A g^{-1}）	Capacity（mAh g^{-1}）	Cycle numbers	Ref.
Co-based nitrides					
CoN film	0.12	0.0825	1000	80	[1]
Porous CoN	-	0.248	650	60	[2]

CoN	1.44	0.06	956	60	[3]
CoN	-	0.5	750	150	[4]
Co-based oxides					
porous hollow Co_3O_4	-	0.1	1100	50	[5]
Co_3O_4 @N-C	1.37	0.5	795	300	[6]
Porous Co_3O_4 Nanofoils	-	0.89	1000	100	[7]
Co_3O_4@CNT	-	0.1	700	60	[8]
Co_3O_4 Rose-Spheres	-	0.09	990	100	[9]
Hollow Co_3O_4	-	0.05	880	50	[10]
C-doped Co_3O_4 HNFs	1	0.2	1121	100	[11]
Mesoporous Co_3O_4	-	0.89	600	300	[12]
MWCNTs/Co_3O_4	-	0.1	813	100	[13]
Mesoporous Co_3O_4	-	0.2	913	60	[14]
Co-based sulfides					
Co_9S_8/$Co_{1-x}S$@NC	1.68	0.05	1230	100	[15]
Co_9S_8/MoS_2	-	1	756	70	[16]
Hollow Co_9S_8	1.5	0.544	366	150	[17]
Co_9S_8 nanorods	1	0.1	540	300	[18]
Hollow CoS_x	1	0.5	572	100	[19]
om-CoN	1.4	1	710	350	Our work
		2	300	2000	

4. Supplementary References

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