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

Cobalt Nickel Nitride Coated by Thin Carbon Layer Anchoring on Nitrogen-Doped Carbon Nanotubes Anodes for High-Performance Lithium-Ion Batteries

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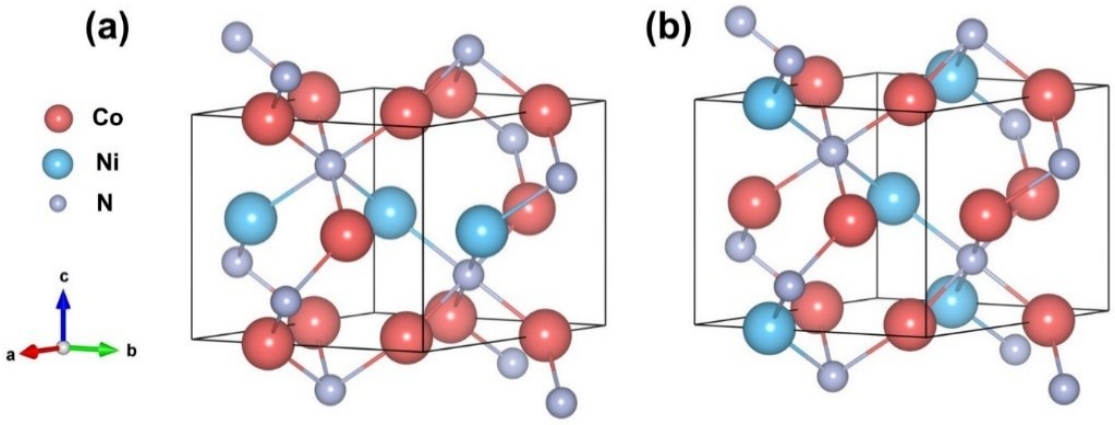

Figure S1. Two possible arrangements of $NiCo_2N$ in $P6_322$ point symmetry. (a) The Ni possessed the nearby octahedral position regarding to central N. (b) The Ni possessed the far away octahedral positions regarding to central N. The red, blue and purple balls represent Co, Ni and N atoms.

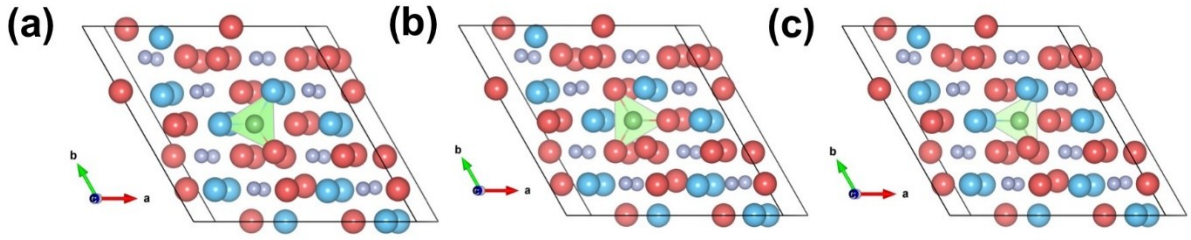

Figure S2. Li atom in two different bonding sites (a) and (b) in path A direction, denoted as A_a and A_b, respectively. And (a) and (c) are identical site. The diffusive energy of path A was calculated by Li atom diffuse from (a), through (b) to (c).

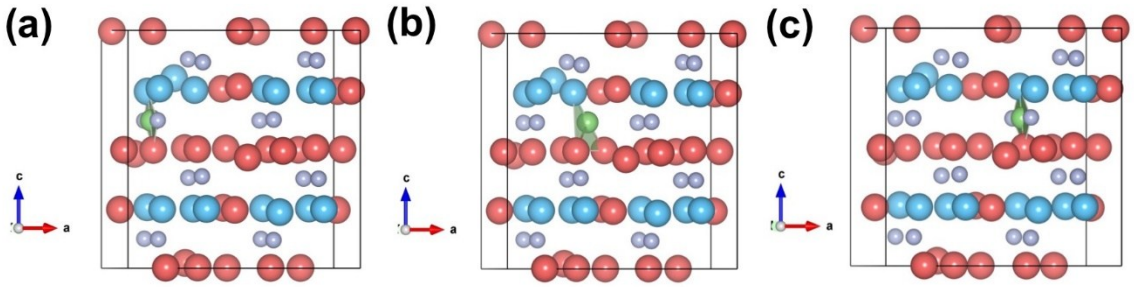

Figure S3. Li atom in two different bonding sites (a) and (b) in path B direction, denoted as B_a and B_b, respectively. And (a) and (c) are identical sites. The diffusive energy of path A was calculated by Li atom diffuse from (a), through (b) to (c).

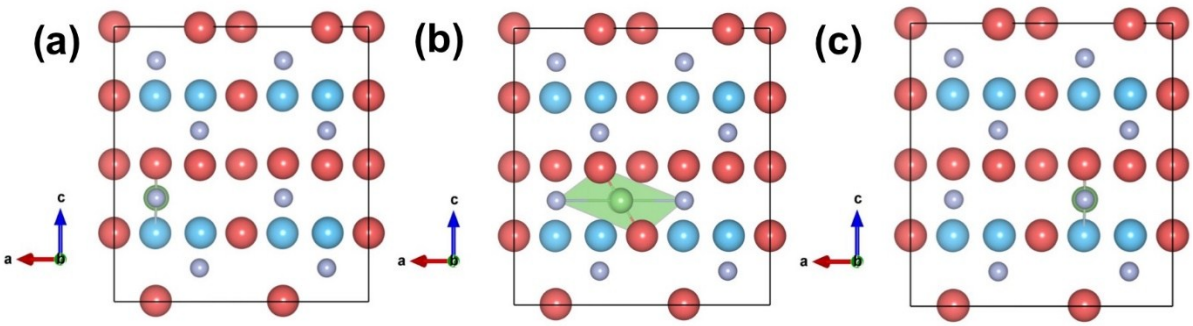

Figure S4. Li atom in two different bonding sites (a) and (b) in path C direction, denoted as C_a and C_b, respectively. And (a) and (c) are identical site. The diffusive energy of path A was calculated by Li atom diffuse from (a), through (b) to (c).

The coordinates of the primary cell of $NiCo_2N$

$NiCo_2N$
1.00000000000000
4.5845929390000002 0.0000000000000000 0.0000000000000000
-2.2922964700000001 3.9702574849999999 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.2723599559999998
Co Ni N
4 2 2
Direct
0.3264896160144914 -0.0026462494330634 -0.0060090561330398
-0.0000103702809980 0.3305527643887258 0.9999262808916037
0.6735529299251191 0.6709503708015288 0.0060495139009422
0.9999894476502686 0.6700847050978436 0.5000281913114299
0.3222004549841393 0.3232172993764738 0.5011085535980648
0.6777153135361291 0.0010354581729377 0.4988710852792609
0.3305655827992935 0.6686763100346782 0.2452808153848053
0.6694969953715547 0.3381293415608759 0.7547446157669329

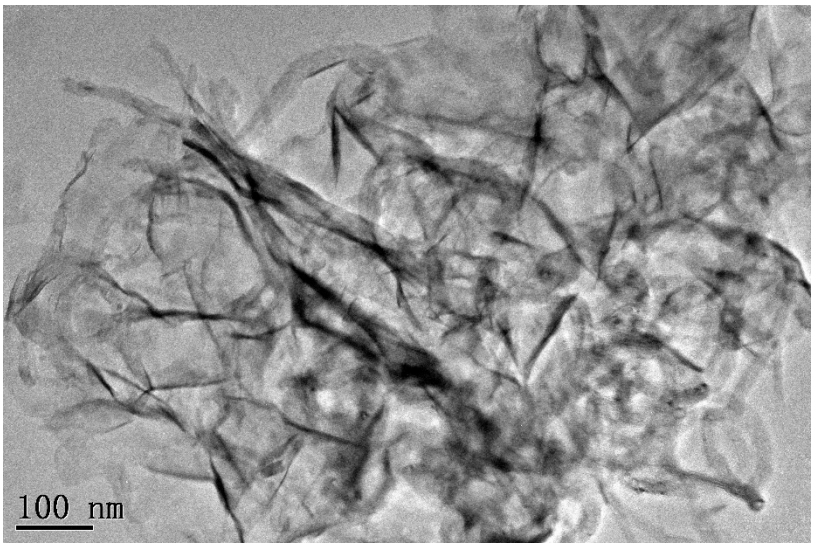

Figure S5. TEM image of the NiCo-precursor-NCNTs nanocomposite.

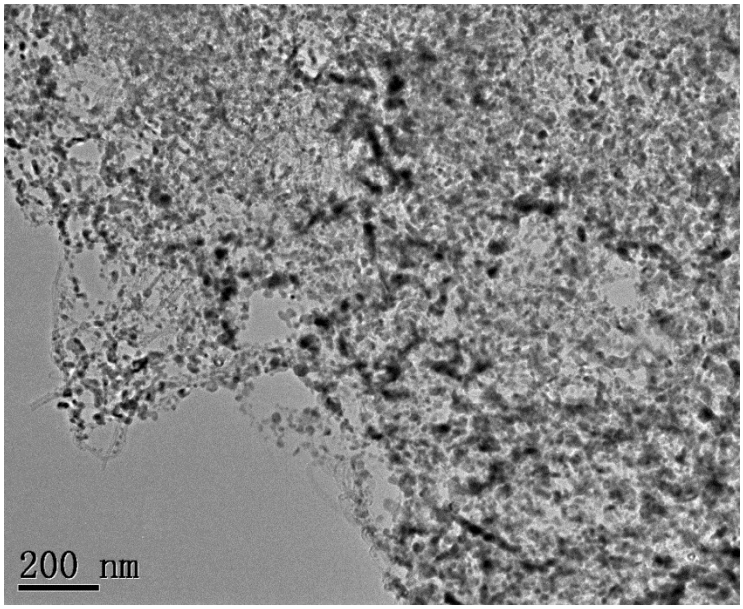

Figure S6. Low magnification TEM image of the $NiCo_2N$@C-NCNTs nanocomposites.

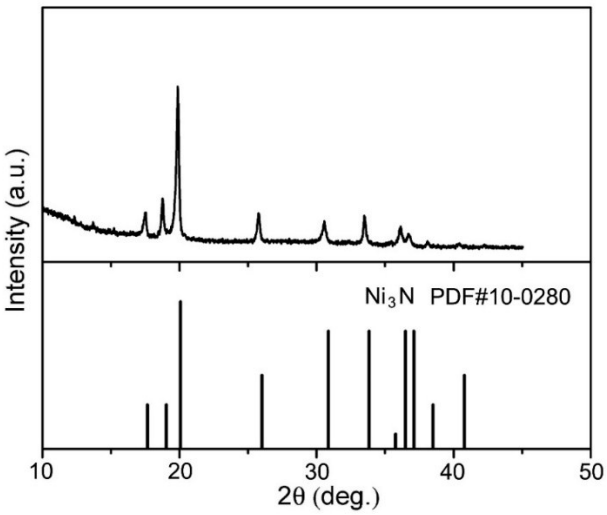

Figure S7. XRD patterns of the $NiCo_2N$@C-NCNTs nanocomposite (upper panel) and JCPDS card (Ni_3N, No. 10-0280) (lower panel).

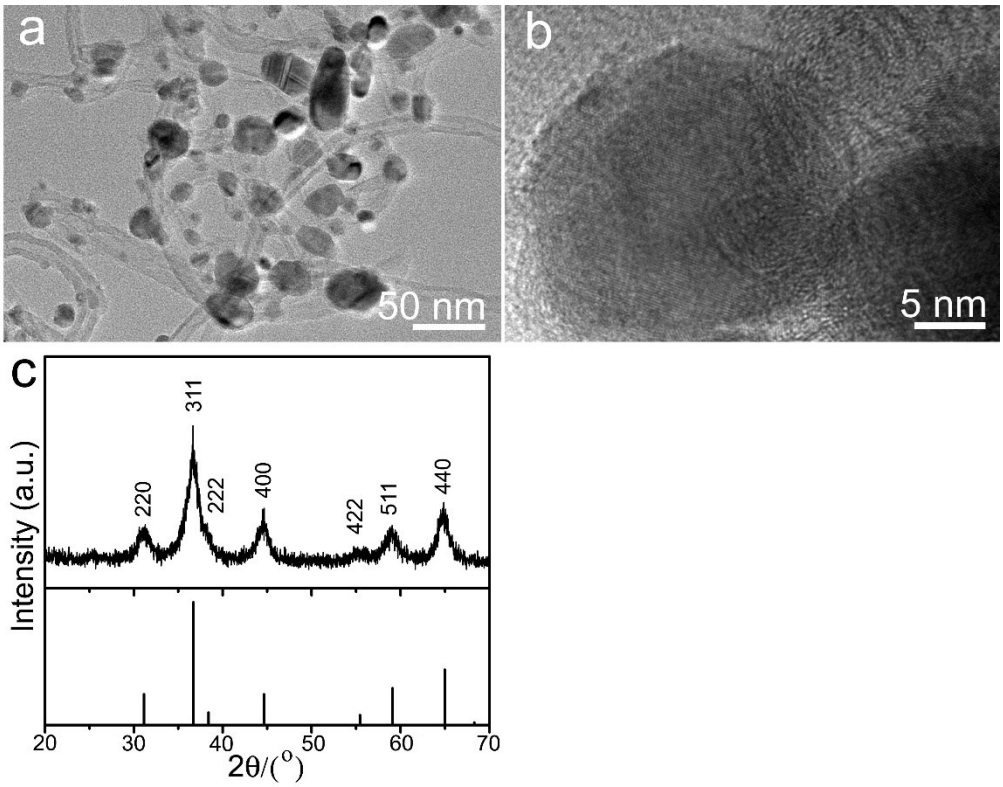

Figure S8. (a) TEM, (b) HRTEM and (c) XRD images of the $NiCo_2O_4$-NCNTs nanocomposite.

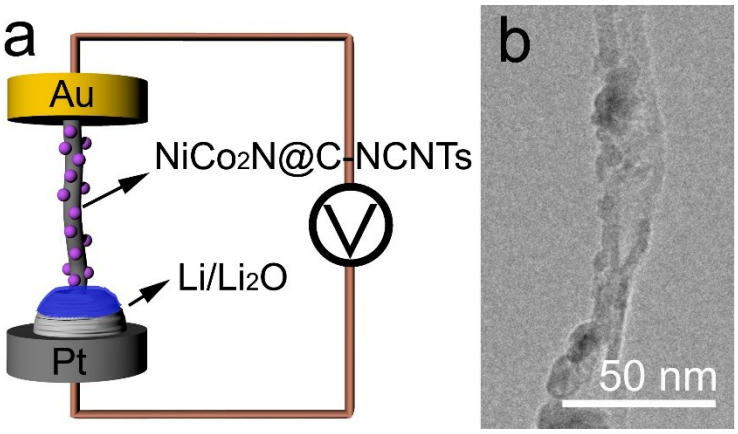

Figure S9. A schematic diagram of the in-situ TEM experiment procedure of an all solid nanobattery cell constructed inside a TEM. A $NiCo_2N$@C-NCNTs nanocomposite is placed on a Au wire, serving as the working electrode; the counter-electrode consisted of a small piece of Li metal coated with Li_2O (solid electrolyte) on the tip of a Pt wire. A bias voltage of -3/3 V was applied between the two electrodes to drive the lithiation delithiation process.

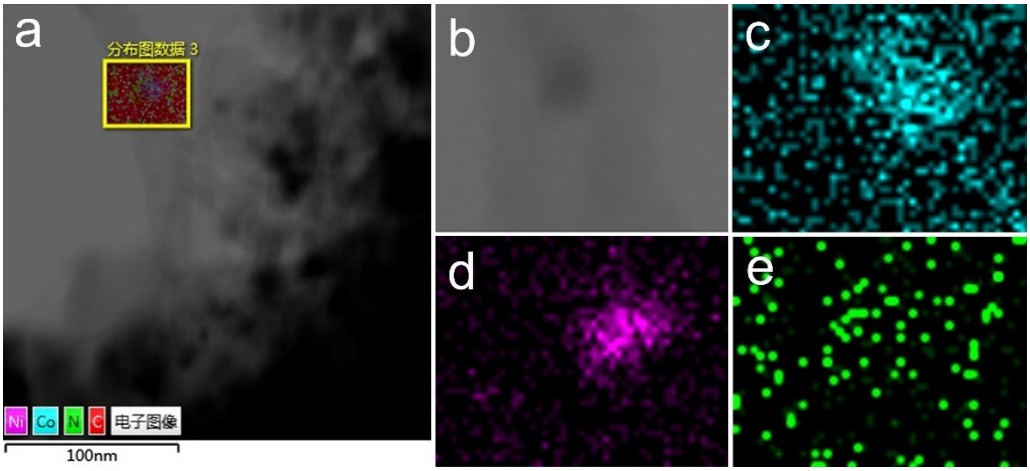

Figure S10. EDX elemental mapping show Co (c), Ni (d), and N elements inside NCNT.

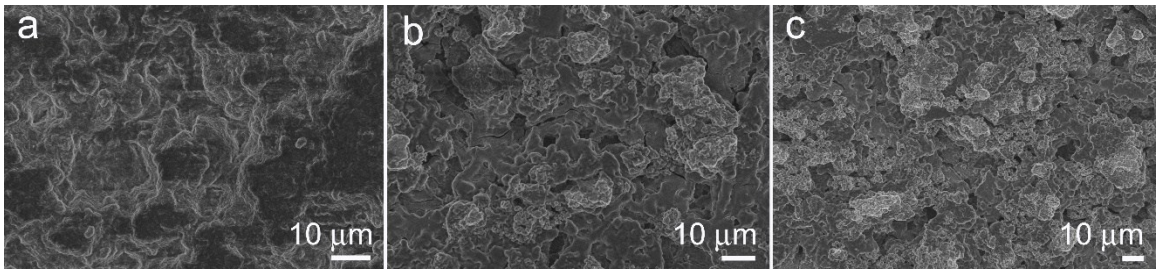

Figure S11. SEM images of $NiCo_2N$@C-NCNTs nanocomposite after test for (a) 150th cycle, (b) 250th cycle and (c) 500th cycle at the high current density of 2000 mA g^{-1}.

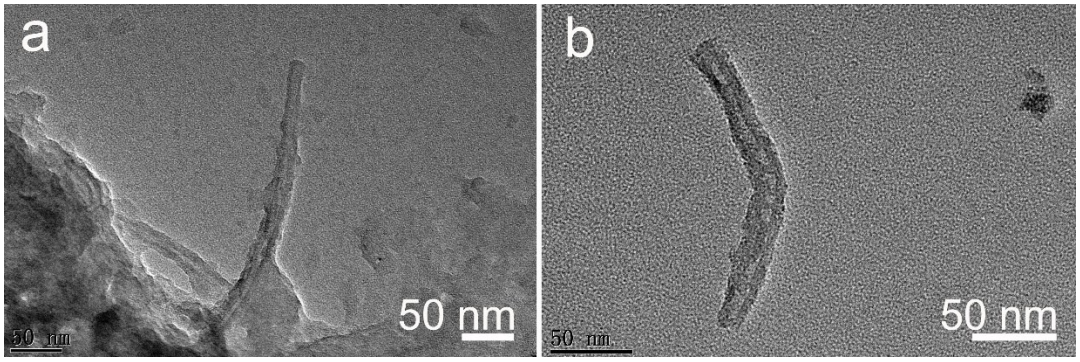

Figure S12. TEM images of $NiCo_2N$@C-NCNTs nanocomposite after test for (a) 250th cycle and (b) 500th cycle at the high current density of 2000 mA g^{-1}.