Three-dimensional self-supported $CuCo_2O_4$ nanowires@NiO nanosheets core/shell arrays as an oxygen electrode catalyst for Li-O_2 batteries

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DFT calculation models: The present first principle density functional theory calculations are performed by Vienna Ab initio Simulation Package with the projector augmented wave method. The exchange-functional is operated by utilizing the generalized gradient approximation of Perdew-Burke-Ernzerhof functional. To optimize cell optimization and calculations of atoms, the cut-off energy of the plane-wave basis is recorded at 450 eV. The vacuum spacing in a direction perpendicular to the plane of the catalyst is at least 20 Å. The Brillouin zone integration is conducted to use 2x2×1 Monkhorst-Pack k-point sampling for a primitive cell. A convergence energy threshold of 10^{-5} eV is applied in the self-consistent calculations. The equilibrium lattice constants are optimized with maximum stress on each atom within 0.05 eV/Å.

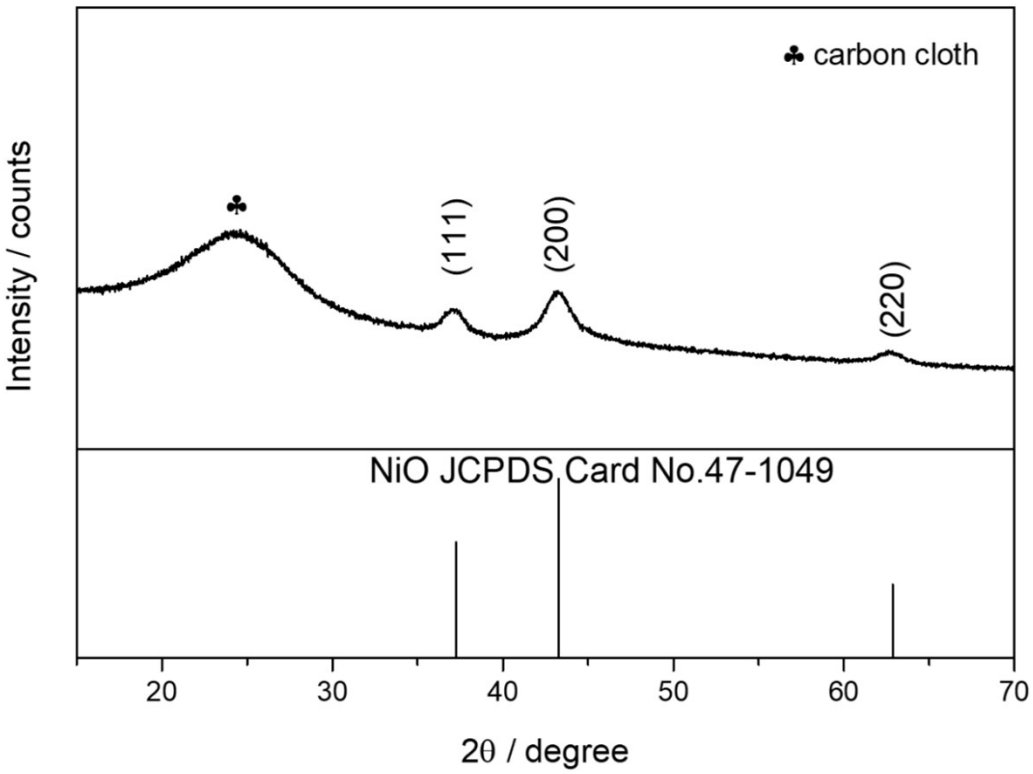

Fig. S1 XRD patterns of the NiO/CC.

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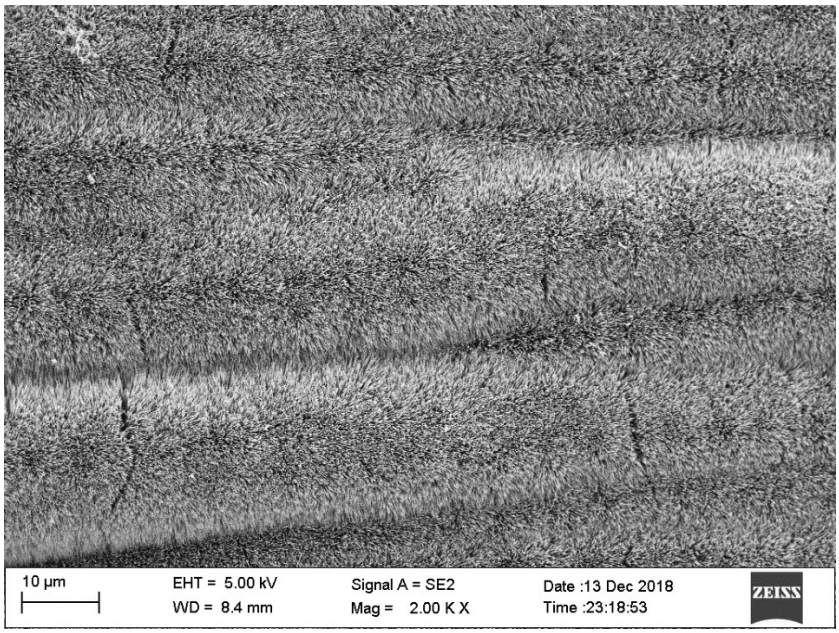

Fig. S2 FE-SEM images of the $CuCo_2O_4$/CC.

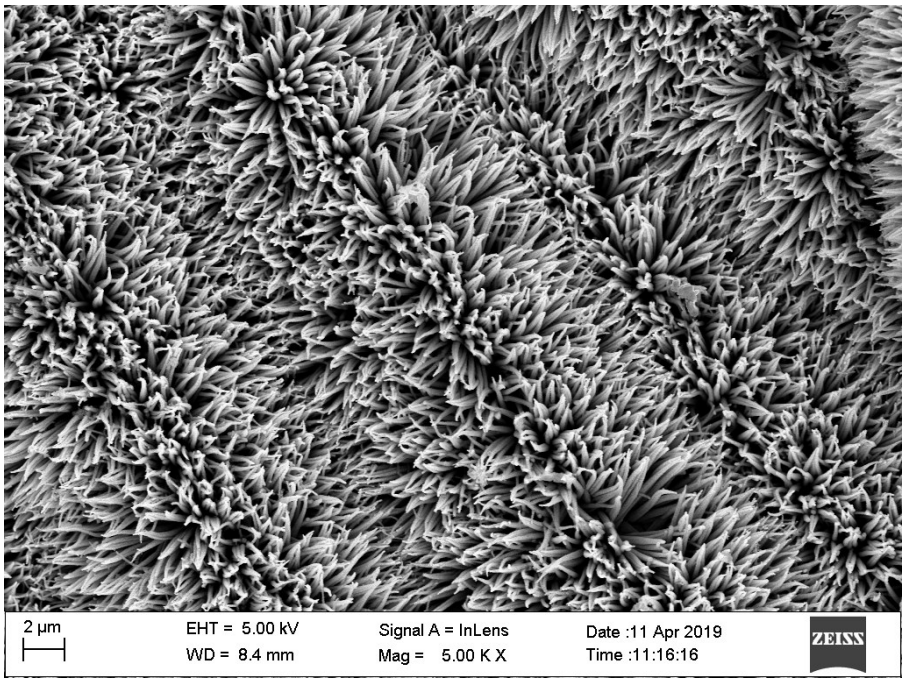

Fig. S3 FE-SEM images of the $CuCo_2O_4$@NiO/CC.

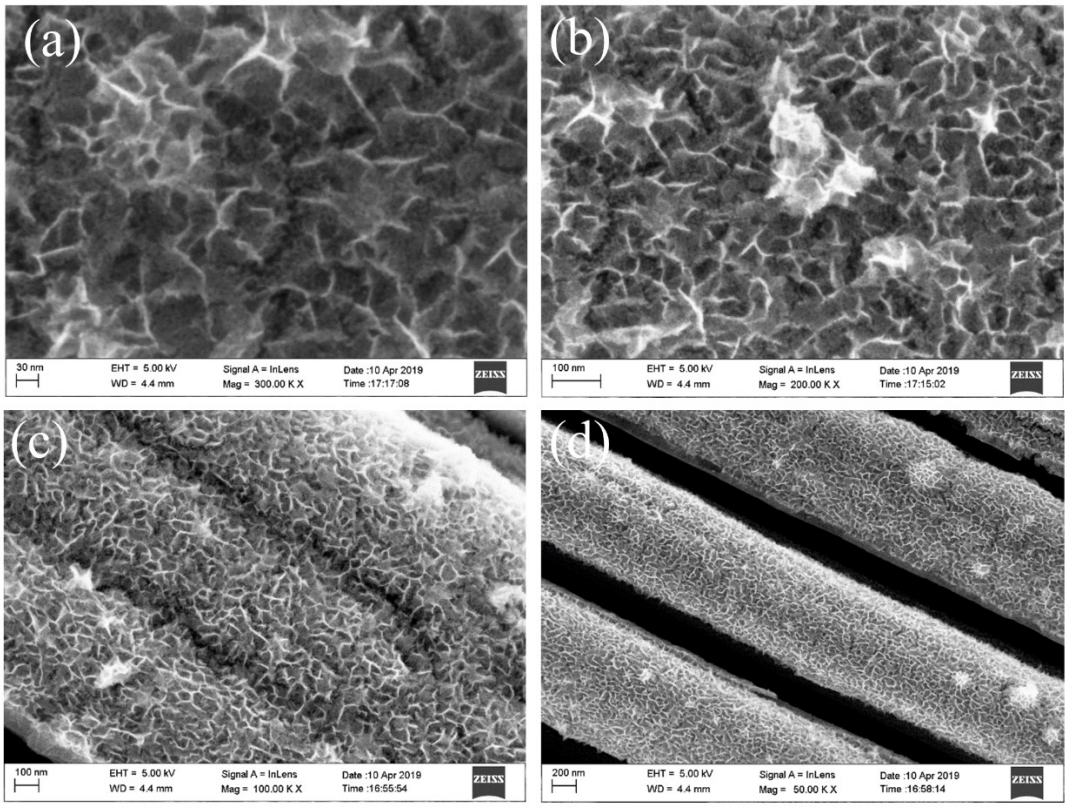

Fig. S4 FE-SEM images of the NiO/CC.

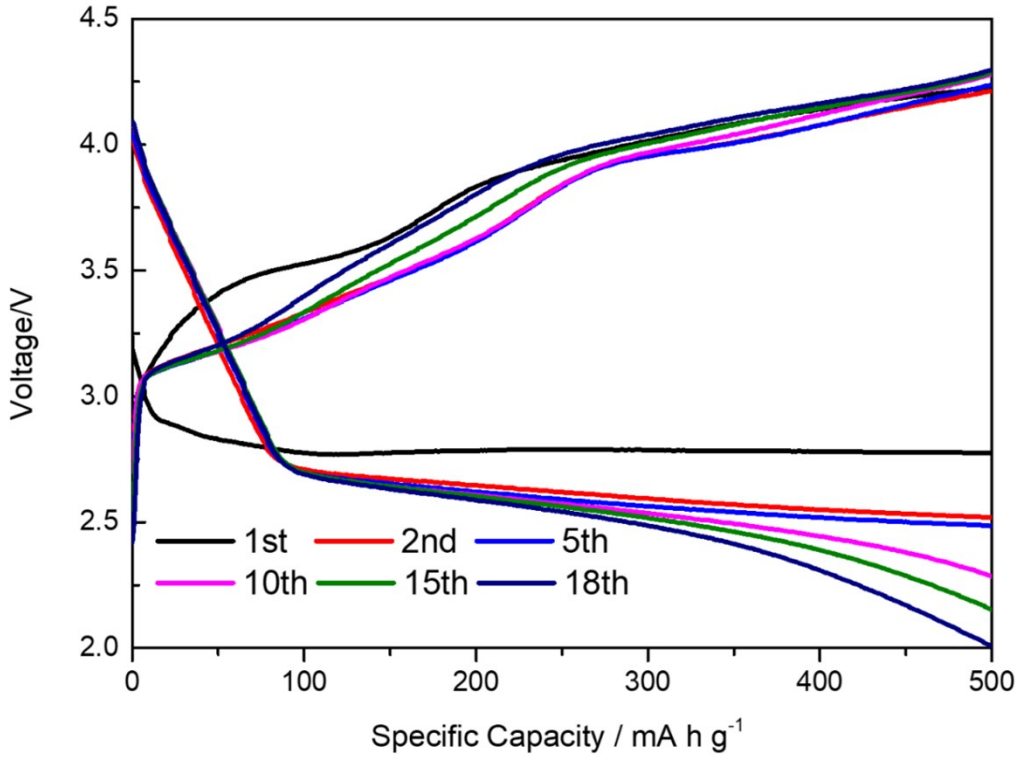

Fig. S5 The discharge and charge curves of LOBs with the NiO/CC under a limited capacity of 500 mA h g^{-1} at 0.2 mA cm^{-2}.

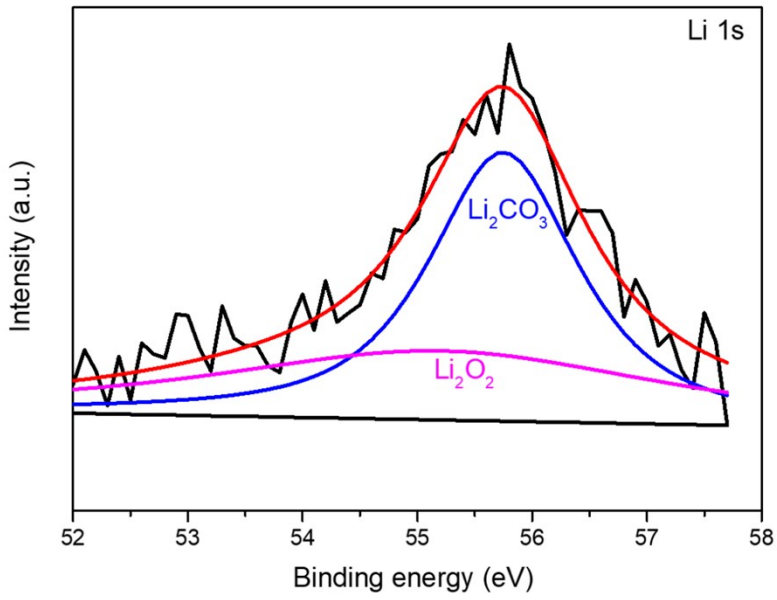

Fig. S6 The ex-situ XPS spectra of $CuCo_2O_4$@NiO/CC cathode after first overcharge (The charge specific capacity of 11721 mA h g^{-1} exceeds the corresponding discharge specific capacity of 9335 mA h g^{-1}) in Li 1s regions at 0.2 mA cm^{-2}.

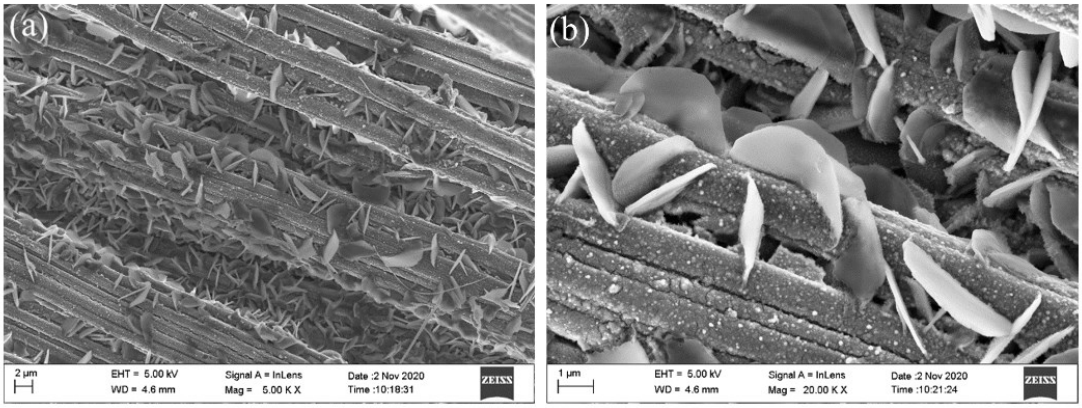

Fig. S7 FE-SEM images for NiO/CC electrode after the 1st cycle discharge. (Under a limited capacity of 2000 mA h g^{-1} at 0.2 mA cm^{-2})

Table S1 Comparison of electrochemical performances of LOBs with $CuCo_2O_4$@NiO/CC and the other reports that use $CuCo_2O_4$ or NiO as the catalysts. (All specific capacities and current densities were calculated based on the total mass loading of catalysts in the electrodes.)

Cathode	Maximum discharge capacity/ current density (~mA h g^{-1}/~mA cm^{-2})	Limited capacity / current density (~mA h g^{-1}/~mA cm^{-2})	Cycle number	Ref
mesoporous $CuCo_2O_4$	7456/0.11	500/0.11	28	S1
$CuCo_2O_4$ nanoparticles	5288/0.057 4687/0.114	500/0.114	85	S2
$CuCo_2O_4$ nanowire/Ni foam	7466/0.5	500/0.1	146	S3
$CuCo_2O_4$ nanosheet/carbon textiles	9970/0.174 8840/0.235	500/0.118	65	S4
Mesoporous NiO	1260/0.059	500/0.059	35	S5
Pt/NiO	2329/0.1	800/0.1	47	S6
Co-Doped NiO/Ni foam	9754/0.168	500/0.168	165	S7
$CuCo_2O_4$@NiO/CC	10843/0.1 9335/0.2 7287/0.3 5179/0.5	500/0.2	181	This work

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