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

Supporting Information

Metal–organic Framework Derived $CoTe_2$ Encapsulated on Nitrogen-doped Carbon Nanotubes Frameworks: High-efficiency Bifunctional Electrocatalyst for Overall Water Splitting

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Characterization

The scanning electron microscopy (SEM) images were observed on a Hitachi S-4800 (Chiyoda-ku, Tokyo, Japan) operated under high vacuum with an accelerating voltage of 7 kV. Transmission electron microscopy (TEM) images and high resolution transmission electron microscopy (HRTEM) images were recorded on a FEI (TecnaiTM F30, USA) microscope with capabilities for energy-dispersive X-ray spectroscopy (EDX, TECNAI G2, USA) operating at 200 KV. The crystal structure data were acquired on a on a Rigaku D/max-2400 diffractometer, using Cu-Kα radiation as X-ray source in the range of 10-90°. Raman spectra were obtained on Jobin-Yvon LabRam HR80 spectrometer (Horiba Jobin Yvon, Inc.) with 532 nm laser excited. The surface area and pore sizes were measured using the Brunauer–Emmett–Teller (BET) and Barrett–Joyner–Halenda (BJH) methods by utilizing a Tristar II 3020 instrument. XPS measurements were performed on a PHI-5702 instrument equipped with an Mg-Kα source (1253.6 eV) at room temperature under 3×10^{-8} Torr.

OER measurements

The OER activities of all samples were measured on an electrochemical workstation (CHI model 760E, Shanghai Chenhua Instrument Factory, China) and investigated by the linear sweep voltammetry (LSV) method within the range of 1.0 to 1.8 V vs. RHE at a slow scan rate of 5 mV s^{-1}. The working electrodes were scanned several times until the signals were stabilized, and then the data were collected. For all testing, a flow of O_2 was used to purge the electrolyte to ensure the O_2/H_2O equilibrium at 1.23 V. The over-potentials (h) at 10 mA cm^{-2} were calculated as follows: η = E (vs. RHE) - 1.23, considering O_2/H_2O equilibrium at 1.23 V. The Tafel slope was calculated according to the Tafel equation as $\eta = a + b \log|J|$, where η denotes the over-potentials, b denotes the Tafel slope, and J denotes the current density. The stability was tested by means of chronopotentiometry and chronoamperometry measurements. The stability of catalyst was also evaluated by cycling the electrode potential (1.0 V to 1.7 V) for 2000 cycles at 0.2 V s^{-1}, after which the LSVs were recorded. Electrochemical impedance spectra (EIS) were measured in a frequency range from 100 kHz to 0.01 Hz at 5 mV and recorded at 1.50 V in O_2-saturated 1.0 M KOH solution. The electrochemically active surface areas of the samples were investigated from double-layer charging curves using cyclic voltammograms (CVs, 1.09 V to 1.14 V).

HER measurements

The HER activities of all samples were measured on the same electrochemical workstation and investigated by LSVs within the range of -1.0 to 0.2 V vs. RHE at a slow scan rate of 5 mV s^{-1}. 1.0 M KOH or 0.5 M H_2SO_4 (purged with pure N_2)

was used as the electrolyte. The Tafel slope was calculated according to the Tafel equation. The stability was tested by means of chronoamperometry measurements. It was also evaluated by cycling the electrode potential (-0.6 V to 0.2 V) for 2000 cycles at 0.2 V s^{-1}, after which the LSV were recorded.

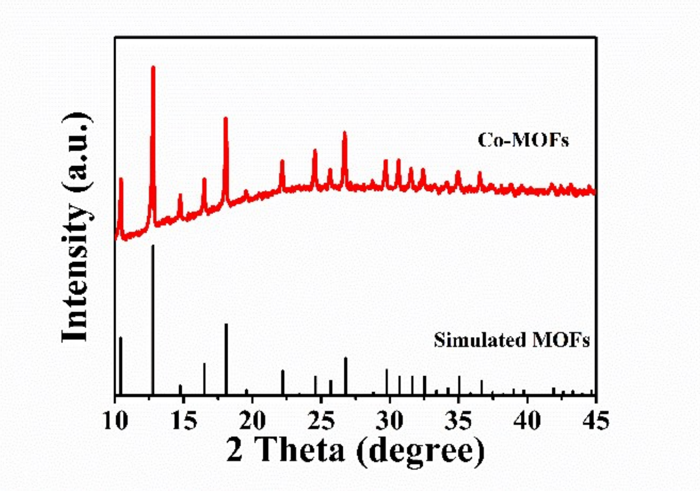

Fig. S1 XRD patterns of ZIF-67.

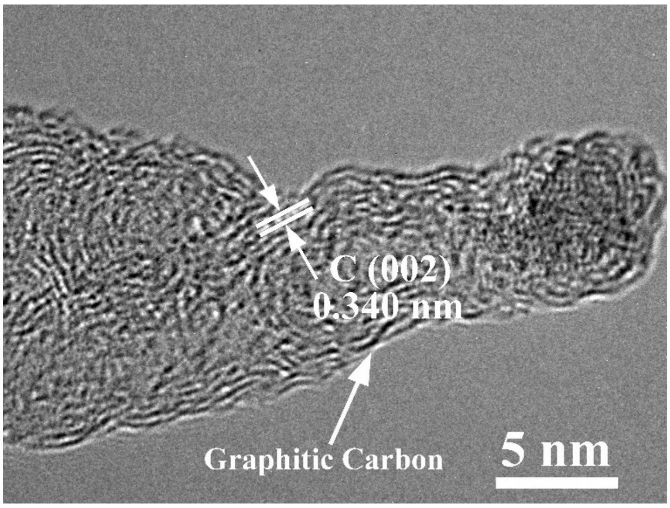

Fig. S2 TEM image of $CoTe_2$@NCNTFs.

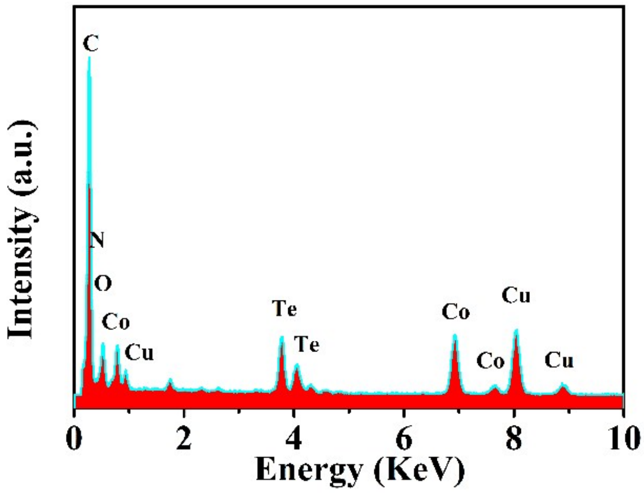

Fig. S3 EDS spectrum of the $CoTe_2$@NCNTFs

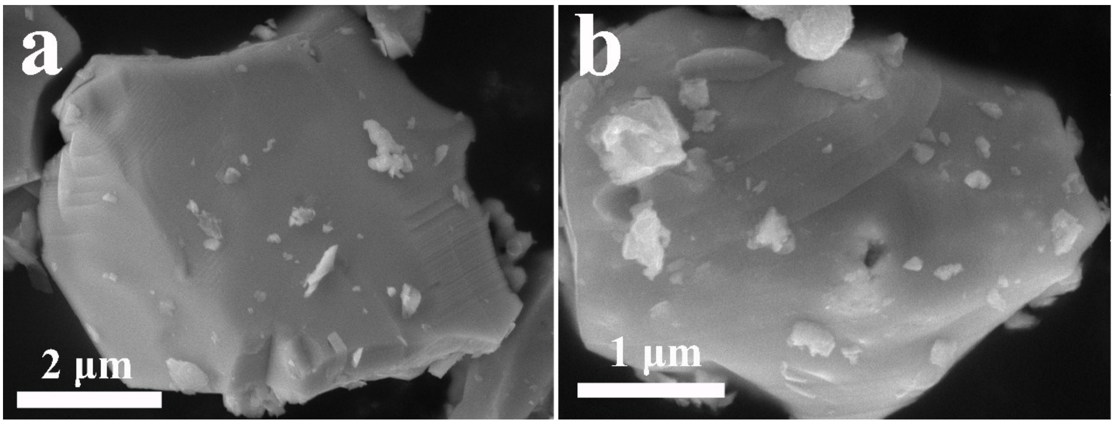

Fig. S4 SEM image of bulk $CoTe_2$.

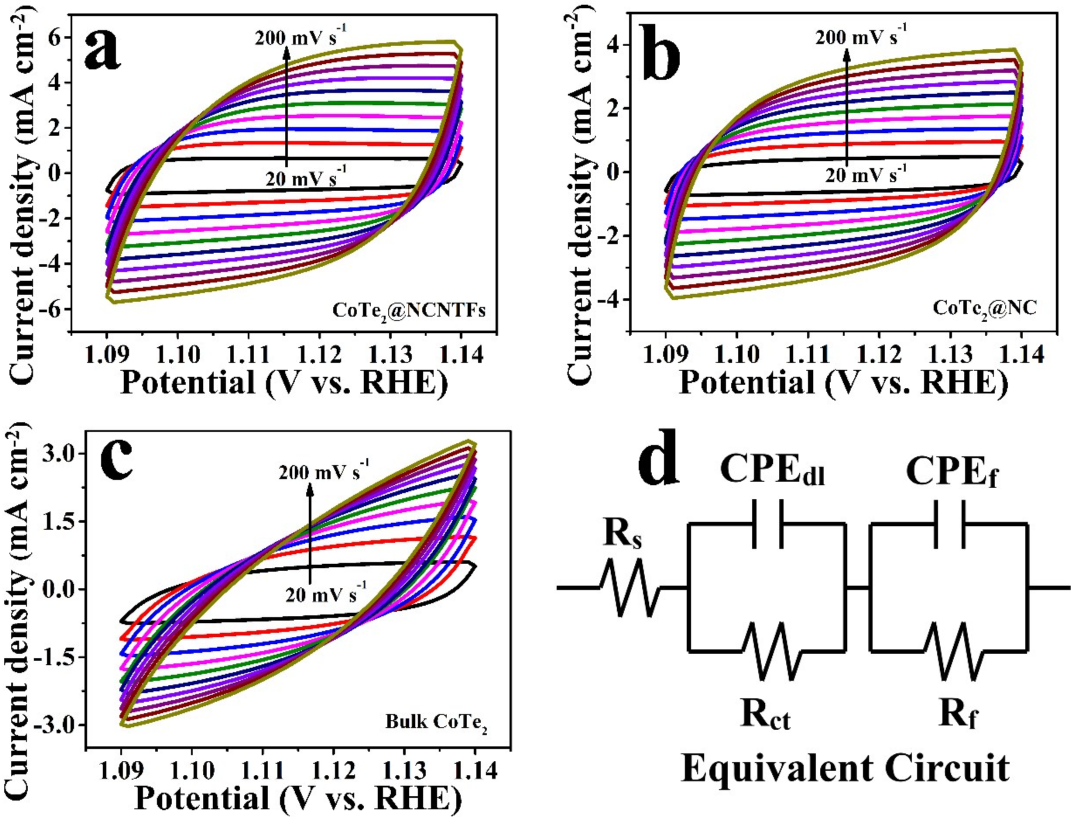

Fig. S5 Voltammograms of the (a) $CoTe_2$@NCNTFs, (b) $CoTe_2$@NC and (c) bulk $CoTe_2$ at various scan rate (20-200 mV s^{-1}) in 1.0 M KOH solution. (d) The equivalent electrical circuit image

Table S1 The atomic percentage distributions of C, N and O in electrocatalysts (C, N and O detected by Elemental Analyzer)

Materials	Elemental composition (at %)		
	C	N	O
$CoTe_2$@NCNTFs-600 ºC	77.74	4.07	7.71
$CoTe_2$@NCNTFs-700 ºC	80.36	3.52	5.34
$CoTe_2$@NCNTFs-800 ºC	83.29	2.96	3.14

Table S2. Comparison of the OER performance of some reported high performance Co-based electrocatalysts in alkaline solution.

Catalysts	Electrolyte	Mass Loading ($mg\ cm^{-2}$)	η^{10} (mV vs. RHE)	Tafel slope ($mV\ dec^{-1}$)	Reference
$CoTe_2$@NCNTFs	1.0 M KOH	0.285	330	82.8	*This work*
$CoTe_2$@N-GC	1.0 M KOH	1.0	300	90	*ACS Appl. Mater. Interfaces.*, 2017, 9, 36146-36153
$CoTe_2$@CoO_x	1.0 M KOH	0.28	380	58	*ACS Catalysis,* 2016, 6, 7393-7397.
$CoTe_2$ Nanofleeces CoTe Nanofleeces	0.1 M KOH 0.1 M KOH	0.25 0.25	357 367	32 73	*Angewandte Chemie*, 2017, 56, 7769-7773
$CoTe_2$/CNT $CoTe_2$ NW	1.0 M KOH 1.0 M KOH	0.405 0.405	291 323	44.2 85.1	*The Journal of Physical Chemistry C*, 2016, 120, 28093-28099.
ECT-Te-CoO ECT-Te-$Co_{0.5}Fe_{0.5}O$ ECT-Te-$Co_{0.37}Ni_{0.26}Fe_{0.37}O$	1.0 M KOH 1.0 M KOH 1.0 M KOH		343 326 276	64.2 39.3 49.6	*Nano Lett*, 2016, 16, 7588-7596
Cu_7Te_4 nanosheets	0.1 M KOH	0.20	460	103	*Nano Energy*, 2017, 41, 780-787
$Zn_{0.1}Co_{0.9}Se_2$	1.0 M KOH	0.285	340	43.2	*J. Mater. Chem. A*. 2017, 5, 17982-17989.
Zn-doped $CoSe_2$/CFC	1.0 M KOH		356	88	*ACS Appl. Mater. Interfaces, 2016, 8, 26902-26907*
$CoSe_2$/CF	1.0 M KOH	2.9	297	41	*Nano Research, 2016, 9, 2234-2243*
$CoSe_2$ $NiSe_2$	1.0 M KOH 1.0 M KOH	1.0 1.0	430 250	50 38	*ACS Appl. Mater. Interfaces. 2016, 8, 5327-5334*
Co-P/NC	1.0 M KOH	0.283	350	52	*Chem. Mater.*, 2015, **27**, 7636-7642
CoP/rGO	1.0 M KOH	0.28	340	66	*Chem. Sci.*, 2016, **7**, 1690-1695
CoP Hollow Polyhedrons	1.0 M KOH	0.102	400	57	*ACS Appl. Mater. Interfaces*, 2016, 8, 2158-2165
PNC/Co	1.0 M KOH	0.35	370	76	*J. Mater. Chem. A*, 2016, 4, 3204-3209
Co@Co3O4/NC	0.1 M KOH	0.21	410	54.3	*Angewandte Chemie*, 2016, 55, 4087-4091
N/Co-doped PCP//NRGO	0.1 M KOH	0.714	430	292	*Adv. Funct. Mater.*, 2015, 25, 872-882
Co@Co_3O_4@NMCC/rGO	1.0 M KOH	0.298	340	71	*Dalton Trans.*, 2016, 45, 5575-5582
Co_3O_4@C-MWCNTs	1.0 M KOH	0.325	320	62	*J. Mater. Chem. A*, 2015, 3, 17392-17402.

Table S3. Comparison of the HER performance of some reported high performance electrocatalysts.

Catalysts	**Electrolyte**	**Mass Loading (mg cm^{-2})**	**η^{10} (mV vs. RHE)**	**Tafel slope (mV dec^{-1})**	**Reference**
$CoTe_2$@NCNTFs	0.5 M H_2SO_4 1.0 M KOH	0.285	240 208	61.67 58.04	*This work*
$CoTe_2$ NP $CoTe_2$ MS	0.5 M H_2SO_4 0.5 M H_2SO_4		246 330	41.0 45.9	*Chem. Commun.*, 2015, 15, 17012-17015
CoTe NSs/$CoTe_2$ NTs CoTe NTs $CoTe_2$ NDs/$CoTe_2$ NTs	0.5 M H_2SO_4 0.5 M H_2SO_4 0.5 M H_2SO_4	4.85 4.57	172 284 309	57.1 58.7 63.2	*ACS Appl. Mater. Interfaces*, 2016, 8, 2910-2916.
$CoTe_2$ $NiTe_2$	0.5 M H_2SO_4 0.5 M H_2SO_4	0.028 0.028	580 560	51.0 44.0	Chem. Eur. J. 2017, 23, 11719-11726
PNC/Co	1.0 M KOH	0.35	298	131	*J. Mater. Chem. A*, 2016, 4, 3204-3209
CoP/rGO	0.5 M H_2SO_4 1.0 M KOH	0.283	105 150	50 38	*Chem. Sci.,* 2016, 7, 1690-1695
Co_2P@N, P-PCN/CNTs	0.5 M H_2SO_4 1.0 M KOH	0.36	126 154	45 52	*J. Mater. Chem. A*, 2016, 4, 15501-15510
CoP/CC	0.5 M H_2SO_4 1.0 M KOH	0.92	67 209	51 129	*J. Am. Chem. Soc.*, 2014, 136, 7587-7590
Co-NRCNTs	0.5 M H_2SO_4 1.0 M KOH	0.28	260 370	69	*Angew. Chem. Int. Ed.* *2014, 53, 4372-4376*
MoB	0.5 M H_2SO_4 1.0 M KOH		215 225	55 59	*Angew. Chem. Int. Ed.* *2012, 51, 12703.*
Ni_2P/NiCoP@NCCs	0.5 M H_2SO_4 1.0 M NaOH	0.5	120 116	90 79	*J. Mater. Chem. A,* 2017, 5, 16568-16572.
NiP_2 NS/CC	0.5 M H_2SO_4 1.0 M KOH	2.6	152 102	51 65	*Nanoscale,* *2014, 6, 13440-13445*

Table S3 Comparison of electrocatalytic performance of $CoTe_2$@NCNTFs with other reported bifunctional electrocatalysts for overall water splitting in a two-electrode cell.

Catalyst	**Electrolyte**	**Mass Loading ($mg\ cm^{-2}$)**	**Voltage@10 mA cm^{-2} (V)**	**Reference**
$CoTe_2$@NCNTFs	1.0 M KOH	1.0	1.67	*This work*
PNC/Co	1.0 M KOH	1.0	1.64	*J. Mater. Chem. A*, 2016, 4, 3204-3209
Co_2P@N, P-PCN/CNTs	1.0 M KOH	1.0	1.64	*J. Mater. Chem. A*, 2016, 4, 15501-15510
a-CoSe/Ti	1.0 M KOH	3.8	1.65	*Chem. Commun., 2015, 51, 16683*
$CoSe_2$/CF	1.0 M KOH	2.9	1.63	*Nano Res., 2016, 9, 2234-2243.*
Co-P/NC	1.0 M KOH		1.71	*Chem. Mater.*, 2015, **27**, 7636-7642
CoP/rGO	1.0 M KOH	0.28	1.70	*Chem. Sci.*, 2016, **7**, 1690-1695
$NiCo_2S_4$ NA/CC	1.0 M KOH	4.0	1.68	*Nanoscale*, 2015, **7**, 15122-15126
NiSe/Ni foam	1.0 M KOH	2.8	1.63	*Angew. Chem. Int. Ed.*, 2015, 54, 9351-9355
Ni_5P_4	1.0 M KOH	1.74	1.70	*Angew. Chem. Int. Ed.*, 2015, 54, 12361-12365.
NiFe LDH/Ni foam	1.0 M KOH		1.70	*Science*, 2014, 345, 1593-1596