Electronic Supplementary Information:

Micron-Sized Hexagonal Single-Crystalline Rods of Metal Nitride Clusterfullerene: Preparation, Characterization, and Photoelectrochemical Application

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S1: **SEM image of micron-sized needle-like rods prepared by LLIP method using *m*-xylene as solvent dissolving $Sc_3N@C_{80}$.**

3 mL isopropanol was slowly added into 1 mL 0.6 mg/mL $Sc_3N@C_{80}$ solution in *m*-xylene in a 5 ml glass vessel to keep a placid interface between *m*-xylene and isopropanol. The sample vessel was shaken by hand for 1 min, then followed by ultrasonication for 5 min to form plenty of small microbubbles. After ultrasonication, the mixture was kept at room temperature for 12 h.

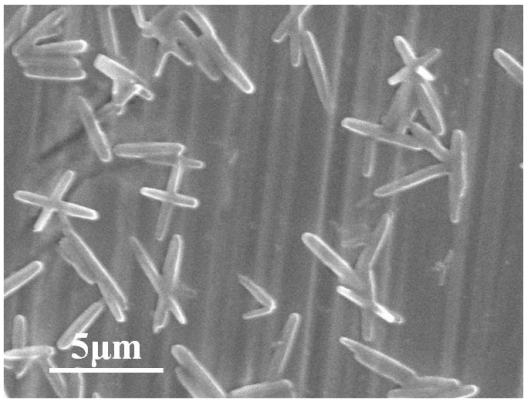

Fig S1: SEM image of micron-sized needle-like rods prepared by LLIP method using *m*-xylene as solvent dissolving $Sc_3N@C_{80}$.

S2: **SEM image of $Sc_3N@C_{80}$ rods with messy shapes obtained without shaking prior to ultrasonication.**

3 mL isopropanol was slowly added into 1 mL $Sc_3N@C_{80}$ solution in *p*-xylene with variable concentrations in a 5 ml glass vessel to keep a placid interface between *p*-xylene and isopropanol. Then the sample was ultrasonicated for 5 min kept at room temperature for 12 h.

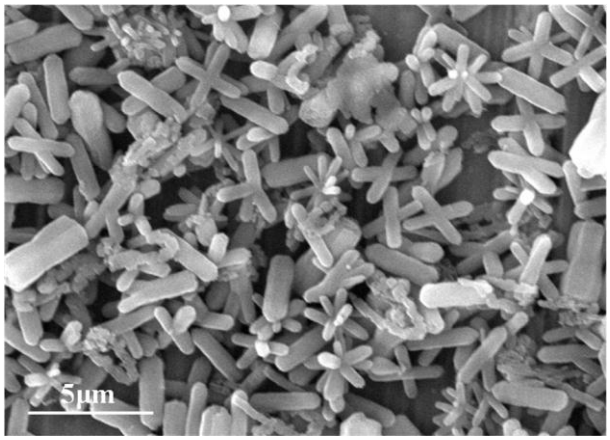

Fig. S2: SEM image of $Sc_3N@C_{80}$ rods with messy shapes.

S3: **Selected area electron diffraction (SAED) pattern of $Sc_3N@C_{80}$ rods with distinct three-order diffraction of d-spacings of 28.6 Å, 14.2 Å and 9.5 Å.**

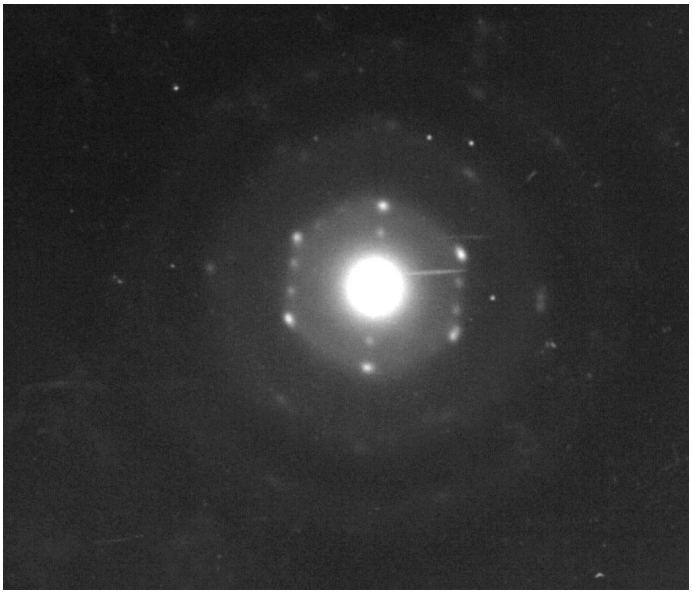

Fig. S3: Selected area electron diffraction (SAED) pattern of $Sc_3N@C_{80}$ rods with distinct three-order diffraction.

S4: **Detailed indexing data of $Sc_3N@C_{80}$ crystals with the assigned hexagonal system in comparison with the assumed orthogonal system.**

(I) Crystal system: **Hexagonal Lattice** Type: P

Lattice Parameter: a= 33.05 b= 33.05 c= 18.4

Lattice Parameter: Alpha= 90 Beta= 90 Gama=120

Radiation: Cu WaveLength: 1.540598

2Theta Start= 0.8 2Theta End= 30

Total 170 Lines are generated!

H	K	L	d	2Theta					
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1	1	0	16.525	5.344	3	0	1	8.46982	10.436
1	0	1	15.47767	5.705	2	2	0	8.2625	10.699
2	0	0	14.31107	6.171	1	1	2	8.03823	10.998
1	1	1	12.29456	7.184	3	1	0	7.93835	11.137
2	0	1	11.29649	7.82	2	0	2	7.73884	11.425
2	1	0	10.81815	8.166	2	2	1	7.53743	11.731
3	0	0	9.54071	9.262	3	1	1	7.28893	12.133
2	1	1	9.32573	9.476	4	0	0	7.15553	12.36
					2	1	2	7.00838	12.62

4	0	1	6.66899	13.265
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3	2	0	6.56637	13.474
4	1	0	6.24586	14.169
3	2	1	6.18436	14.31
2	2	2	6.14728	14.397
0	0	3	6.13333	14.43
3	1	2	6.01022	14.727
1	0	3	5.99719	14.759
4	1	1	5.91441	14.967
1	1	3	5.75006	15.397
5	0	0	5.72443	15.467
4	0	2	5.64824	15.677
2	0	3	5.63742	15.707
3	3	0	5.50833	16.077
5	0	1	5.46601	16.203
4	2	0	5.40908	16.374
3	2	2	5.34466	16.573
2	1	3	5.33549	16.602
3	3	1	5.27695	16.787
4	2	1	5.18949	17.072
4	1	2	5.16752	17.146
3	0	3	5.15922	17.173
5	1	0	5.14069	17.236
5	1	1	4.95109	17.901
2	2	3	4.92479	17.997
5	0	2	4.86037	18.238
3	1	3	4.85347	18.264
6	0	0	4.77036	18.585
3	3	2	4.726	18.761
4	3	0	4.70545	18.844
4	2	2	4.66286	19.018
4	0	3	4.65677	19.043
6	0	1	4.61769	19.205
0	0	4	4.6	19.28
5	2	0	4.58321	19.351
4	3	1	4.55874	19.456
1	0	4	4.54172	19.53
5	1	2	4.48763	19.767
3	2	3	4.4822	19.792
5	2	1	4.44732	19.948
1	1	4	4.43151	20.02
2	0	4	4.37933	20.261
4	1	3	4.37616	20.276
6	1	0	4.36484	20.329
6	1	1	4.24698	20.9
6	0	2	4.23491	20.96
2	1	4	4.2332	20.969
4	3	2	4.1893	21.191
5	0	3	4.18488	21.214
3	0	4	4.14353	21.428
4	4	0	4.13125	21.492
5	2	2	4.10234	21.645
3	3	3	4.09819	21.668
5	3	0	4.08888	21.718
7	0	0	4.08888	21.718
4	2	3	4.05681	21.891
4	4	1	4.0309	22.034
2	2	4	4.01911	22.099
5	3	1	3.99151	22.254
7	0	1	3.99151	22.254
3	1	4	3.98007	22.319
6	2	0	3.96918	22.381
6	1	2	3.94352	22.528
5	1	3	3.93983	22.55
6	2	1	3.87993	22.903
4	0	4	3.86942	22.966
7	1	0	3.79109	23.447
4	4	2	3.76872	23.588
3	2	4	3.76751	23.596
6	0	3	3.7655	23.608
7	0	2	3.73646	23.795
5	3	2	3.73646	23.795
4	3	3	3.73333	23.815
7	1	1	3.7131	23.946
4	1	4	3.70388	24.007
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5	2	3	3.67139	24.223
5	4	0	3.66469	24.268
1	0	5	3.64996	24.367
6	2	2	3.64446	24.404
6	3	0	3.60605	24.668
5	4	1	3.5941	24.752
1	1	5	3.59201	24.766
5	0	4	3.58574	24.81
8	0	0	3.57777	24.866
2	0	5	3.56405	24.964
6	1	3	3.55623	25.02

6	3	1	3.53873	25.145
3	3	4	3.53075	25.203
8	0	1	3.51199	25.34
7	1	2	3.50516	25.39
4	2	4	3.50419	25.397
7	2	0	3.49675	25.452
2	1	5	3.48394	25.547
7	2	1	3.43527	25.916
3	0	5	3.43344	25.93
5	1	4	3.42797	25.972
4	4	3	3.42645	25.983
5	4	2	3.40453	26.154
7	0	3	3.40215	26.172
5	3	3	3.40215	26.172
2	2	5	3.36165	26.493
6	3	2	3.35736	26.528
8	1	0	3.34997	26.587
3	1	5	3.3387	26.679
8	0	2	3.3345	26.713
6	2	3	3.33227	26.731
6	0	4	3.31128	26.904
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8	1	1	3.29579	27.033
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7	2	2	3.26862	27.262
5	5	1	3.25294	27.396
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6	4	1	3.23213	27.575
7	1	3	3.22478	27.64
7	3	0	3.22024	27.679
3	2	5	3.21023	27.767
9	0	0	3.18024	28.035
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4	1	5	3.17059	28.122
6	1	4	3.16628	28.161
8	1	2	3.14778	28.33
5	4	3	3.1459	28.347
9	0	1	3.13377	28.459
8	2	0	3.12293	28.56
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6	3	3	3.10858	28.695
5	0	5	3.09553	28.818
6	4	2	3.09218	28.85
8	0	3	3.0904	28.867
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4	4	4	3.07364	29.028
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1	0	6	3.04921	29.265
4	2	5	3.04261	29.33
7	3	2	3.03943	29.362
7	2	3	3.03774	29.379
1	1	6	3.01519	29.603
9	0	2	3.00572	29.699
6	2	4	3.00511	29.705
6	5	0	3.00042	29.752
9	1	0	3.00042	29.752
2	0	6	2.99859	29.771
5	1	5	2.99231	29.835

(II) Crystal system: Orthorombic Lattice Type: P

Lattice Parameter: a= 28.6 b= 10.8 c= 18.4

Lattice Parameter: Alpha= 90 Beta= 90 Gama=90

Radiation: Cu WaveLength: 1.540598

2Theta Start= 0.5 2Theta End= 30

Total 164 Lines are generated!

H	K	L	d	2Theta
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1	0	1	15.4	5.707
2	0	0	14.3	6.176
2	0	1	11.2	7.824
0	1	0	10.8	8.18
1	1	0	10.1036	8.745
3	0	0	9.53333	9.269
0	1	1	9.31409	9.488
0	0	2	9.2	9.606
1	1	1	8.85628	9.98
1	0	2	8.75802	10.092
2	1	0	8.61826	10.256
3	0	1	8.46465	10.442
2	1	1	7.80458	11.328
2	0	2	7.73708	11.428
4	0	0	7.15	12.369
3	1	0	7.14717	12.374
0	1	2	7.00344	12.629
1	1	2	6.80246	13.004
4	0	1	6.66451	13.274
3	1	1	6.66222	13.279
3	0	2	6.62009	13.364
2	1	2	6.28964	14.069
0	0	3	6.13333	14.43
1	0	3	5.99698	14.76
4	1	0	5.96187	14.847
5	0	0	5.72	15.479
4	1	1	5.67158	15.612
4	0	2	5.64552	15.684
3	1	2	5.64412	15.688
2	0	3	5.63674	15.709
5	0	1	5.46215	16.214
0	2	0	5.4	16.402
0	1	3	5.33331	16.609
1	2	0	5.30625	16.694
1	1	3	5.24293	16.897

0	2	1	5.18147	17.099
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1	2	1	5.09847	17.38
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2	2	0	5.05181	17.541
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2	2	1	4.87154	18.196
5	0	2	4.85766	18.248
6	0	0	4.76667	18.6
3	2	0	4.69859	18.872
0	2	2	4.65705	19.042
4	0	3	4.65524	19.049
3	1	3	4.65446	19.052
6	0	1	4.61434	19.219
0	0	4	4.6	19.28
1	2	2	4.59651	19.295
3	2	1	4.5525	19.483
1	0	4	4.54163	19.53
5	1	2	4.43016	20.027
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6	1	0	4.36082	20.348
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4	1	3	4.27501	20.761
6	1	1	4.24327	20.918
6	0	2	4.23233	20.973
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4	2	1	4.19561	21.159
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3	2	2	4.18446	21.216
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3	0	4	4.14293	21.431
7	0	0	4.08571	21.735
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0	2	3	4.05298	21.912
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6	1	2	3.94055	22.546
5	2	0	3.92663	22.627
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2	2	3	3.89939	22.787

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7	1	0	3.8214	23.258
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7	1	1	3.74156	23.762
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3	2	3	3.7299	23.837
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1	0	5	3.64991	24.367
4	1	4	3.64195	24.421
5	2	2	3.61145	24.631
0	3	0	3.6	24.71
5	0	4	3.58465	24.818
8	0	0	3.575	24.886
6	2	0	3.57358	24.896
1	3	0	3.57181	24.909
2	0	5	3.56388	24.965
6	1	3	3.55405	25.035
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7	1	2	3.52907	25.215
4	2	3	3.5259	25.238
8	0	1	3.50937	25.359
6	2	1	3.50803	25.369
1	3	1	3.50636	25.381
0	2	4	3.50172	25.415
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0	1	5	3.48334	25.552
1	2	4	3.47576	25.608
1	1	5	3.45778	25.744
3	0	5	3.4331	25.932
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5	1	4	3.40214	26.172
2	2	4	3.40123	26.179
7	0	3	3.40033	26.186
8	1	0	3.39389	26.237
2	1	5	3.38438	26.312
3	3	0	3.36787	26.443
0	3	2	3.35247	26.567
8	1	1	3.33759	26.688
8	0	2	3.33226	26.731
6	2	2	3.33111	26.741
1	3	2	3.32968	26.752
3	3	1	3.31284	26.891

6	0	4	3.31004	26.914
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4	0	5	3.27205	27.233
3	1	5	3.27178	27.235
2	3	2	3.26398	27.301
7	2	0	3.2582	27.351
7	1	3	3.24338	27.478
4	3	0	3.21543	27.722
7	2	1	3.20829	27.784
8	1	2	3.18414	27.999
9	0	0	3.17778	28.057
4	3	1	3.16743	28.15
6	1	4	3.16474	28.175
3	3	2	3.16262	28.194
4	2	4	3.14482	28.357
4	1	5	3.13148	28.48
9	0	1	3.13142	28.481
0	3	3	3.1047	28.731
5	0	5	3.09483	28.825
8	0	3	3.08862	28.884
6	2	3	3.0877	28.893
1	3	3	3.08656	28.904
7	2	2	3.07128	29.051
0	0	6	3.06667	29.095
7	0	4	3.05475	29.211
1	0	6	3.04919	29.266
9	1	0	3.04855	29.272
5	3	0	3.04679	29.289
0	2	5	3.04099	29.346
4	3	2	3.03538	29.402
2	3	3	3.03401	29.415
1	2	5	3.02395	29.516
9	1	1	3.00755	29.68
5	3	1	3.00586	29.697
9	0	2	3.00365	29.72
2	0	6	2.99849	29.772
5	2	4	2.98652	29.894
8	2	0	2.98093	29.951

S5: TGA curve of $Sc_3N@C_{80}$ rods

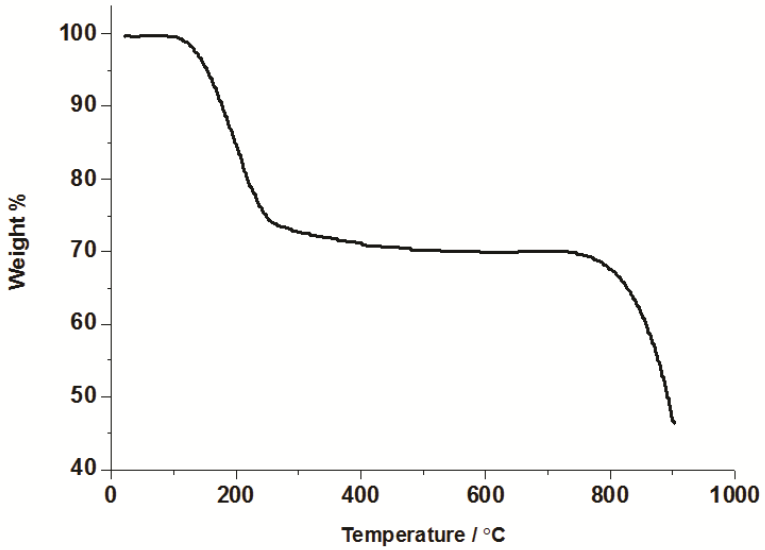

Fig. S4: TGA curve of $Sc_3N@C_{80}$ rods in N_2 atmosphere.

S6: SEM image of $Sc_3N@C_{80}$ rods-modified ITO electrode prepared by electrophoretic deposition

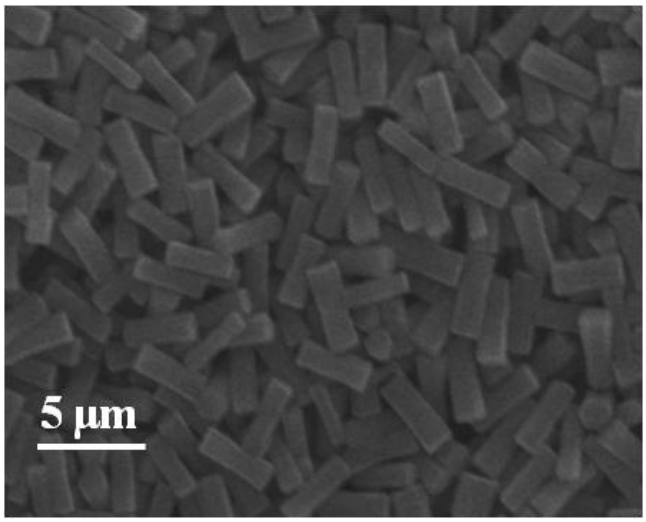

Fig. S5: SEM image of $Sc_3N@C_{80}$ rods-modified ITO electrode prepared by electrophoretic deposition.

S7: UV-vis-NIR spectra of $Sc_3N@C_{80}$ rods-modified ITO electrode prepared by electrophoretic deposition and $Sc_3N@C_{80}$ film drop-coated onto ITO electrode.

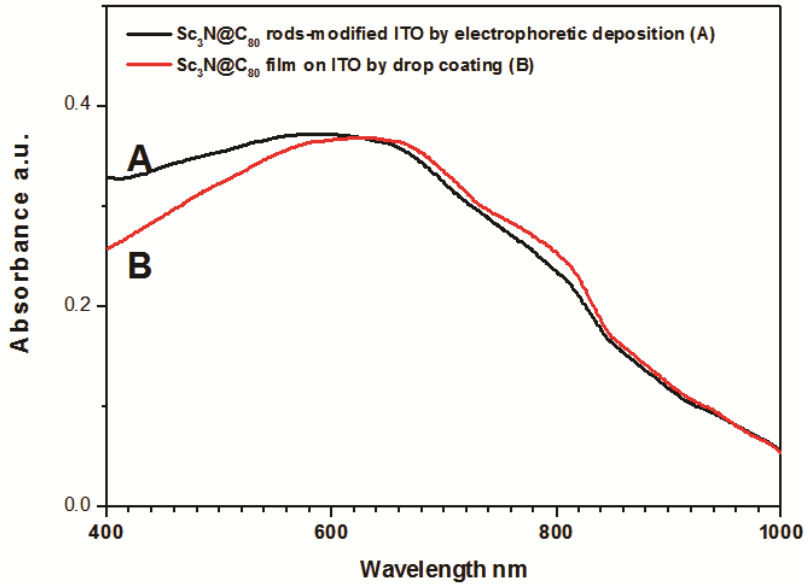

Fig. S6: UV-vis-NIR spectra of $Sc_3N@C_{80}$ rods-modified ITO electrode prepared by electrophoretic deposition (A) and $Sc_3N@C_{80}$ film drop-coated onto ITO electrode (B).