Supplementary material:

Bayesian optimization of wet-impregnated Co-Mo/Al_2O_3 catalyst for maximizing the yield of carbon nanotube synthesis

Sang Su Shin [1,†], Hyeongyun Song [1,†], Yeon Su Shin [1], Jaegeun Lee [1,2,*], and Tae Hoon Seo [3,*]

[1] School of Chemical Engineering, Pusan National University, Busandaehak-ro 63beon-gil, Geumjeoung-gu, Busan 46241, Republic of Korea

[2] Department of Organic Material Science and Engineering, Pusan National University, Busandaehak-ro 63beon-gil, Geumjeoung-gu, Busan 46241, Republic of Korea

[3] Green Energy and Nano Technology & R&D Group, Korea Institute of Industrial Technology (KITECH), Gwangju 61012, Republic of Korea

[†] These authors contributed equally to this work.

[*] Corresponding authors: jglee@pusan.ac.kr (Jaegeun Lee), thseo@kitech.re.kr (Tae Hoon Seo)

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Figure S2. TEM image of as-synthesized CNTs.

Table S1. Predicted and measured value of carbon yield in each iteration when using EI

Iteration number	Metal wt.%	Co wt.%	Mo wt.%	Drying temperature [°C]	Calcination temperature [°C]	Predicted value of carbon yield [%]	Carbon yield [%]
1	61	57	4	123	433	236.4	161.0 ± 4.2
2	70	52	18	80	300	223.6	107.7 ± 14.8
3	59	48	11	154	300	236.8	166.1 ± 8.9
4	42	42	0	183	502	195.2	148.8 ± 5.6
5	40	33	7	142	531	196.6	164.8 ± 6.8
6	70	51	19	124	300	219.6	160.8 ± 16.5
7	58	47	11	108	300	219.9	133.6 ± 6.2
8	48	42	6	145	568	227.6	212.5 ± 18.1
9	66	59	7	151	300	230.0	167.1 ± 6.0
10	45	45	0	129	634	201.9	279.1 ± 15.4
11	46	46	0	139	766	248.4	499.0 ± 21.1
12	46	46	0	138	832	479.9	399.1 ± 24.9
13	46	46	0	164	759	455.1	337.0 ± 17.3
14	51	51	0	134	756	462.4	295.1 ± 8.1
15	44	44	0	134	767	484.7	356.7 ± 12.6
16	47	43	4	136	755	474.4	362.0 ± 10.8
17	47	47	0	143	737	488.7	446.7 ± 8.9
18	46	46	0	125	766	471.0	459.6 ± 15.2
19	49	49	0	91	663	191.6	224.9 ± 3.8
20	49	49	0	93	865	189.1	262.8 ± 5.7
21	56	56	0	95	813	150.2	225.7 ± 4.9
22	52	40	12	93	800	163.9	335.7 ± 44.1
23	53	42	11	117	916	230.2	324.8 ± 17.6
24	55	41	14	127	779	247.9	290.9 ± 14.8

Table S2. Predicted and measured value of carbon yield in each iteration when using OKG

Iteration number	Metal wt.%	Co wt.%	Mo wt.%	Drying temperature [°C]	Calcination temperature [°C]	Predicted value of carbon yield [%]	Carbon yield [%]
1	64	59	5	86	400	230.5	167.8 ± 8.8
2	61	51	10	174	341	232.8	165.9 ± 15.4
3	43	43	0	157	501	220.0	177.5 ± 18.2
4	52	44	8	123	479	226.3	183.2 ± 12.0
5	39	39	0	119	563	217.5	219.6 ± 1.9
6	50	50	0	125	578	220.1	207.1 ± 7.4
7	60	46	14	99	308	224.3	157.7 ± 16.5
8	43	38	5	134	625	204.8	229.8 ± 15.3
9	40	34	6	130	512	214.4	183.5 ± 5.1
10	41	41	0	132	753	221.8	493.6 ± 27.7
11	41	41	0	154	774	472.0	357.4 ± 8.5
12	47	47	0	121	803	476.6	321.4 ± 6.6
13	36	36	0	124	758	473.8	327.2 ± 29.2
14	41	41	0	125	797	465.0	298.7 ± 21.1
15	70	49	21	242	353	91.8	128.7 ± 3.9
16	46	46	0	102	730	491.8	435.7 ± 18.8
17	44	44	0	142	719	487.8	375.2 ± 49.4
18	43	37	6	120	751	456.2	328.4 ± 32.5
19	1	1	0	260	626	54.2	-13.4 ± 3.7
20	50	50	0	131	587	201.4	168.8 ± 2.5
21	48	47	1	96	539	281.5	185.1 ± 5.9
22	40	40	0	119	738	461.2	362.2 ± 8.9
23	50	50	0	133	757	474.9	310.1 ± 11.7
24	38	38	0	138	744	481.2	359.4 ± 1.2

Table S3. Normalized difference between predicted and measured value of carbon yield in each iteration when using EI.

Iteration number	Predicted value of carbon yield [%]	Carbon yield [%]	Normalized difference
1	236.4	161.0 ± 4.2	0.32
2	223.6	107.7 ± 14.8	0.52
3	236.8	166.1 ± 8.9	0.30
4	195.2	148.8 ± 5.6	0.24
5	196.6	164.8 ± 6.8	0.16
6	219.6	160.8 ± 16.5	0.27
7	219.9	133.6 ± 6.2	0.39
8	227.6	212.5 ± 18.1	0.07
9	230.0	167.1 ± 6.0	0.27
10	201.9	279.1 ± 15.4	0.38
11	248.4	499.0 ± 21.1	1.01
12	479.9	399.1 ± 24.9	0.17
13	455.1	337.0 ± 17.3	0.26
14	462.4	295.1 ± 8.1	0.36
15	484.7	356.7 ± 12.6	0.26
16	474.4	362.0 ± 10.8	0.24
17	488.7	446.7 ± 8.9	0.09
18	471.0	459.6 ± 15.2	0.02
19	191.6	224.9 ± 3.8	0.17
20	189.1	262.8 ± 5.7	0.39
21	150.2	225.7 ± 4.9	0.50
22	163.9	335.7 ± 44.1	1.05
23	230.2	324.8 ± 17.6	0.41
24	247.9	290.9 ± 14.8	0.17

Table S4. Normalized difference between predicted and measured value of carbon yield in each iteration when using OKG.

Iteration number	Predicted value of carbon yield [%]	Carbon yield [%]	Normalized difference
1	230.5	167.8 ± 8.8	0.27
2	232.8	165.9 ± 15.4	0.29
3	220.0	177.5 ± 18.2	0.19
4	226.3	183.2 ± 12.0	0.19
5	217.5	219.6 ± 1.9	0.01
6	220.1	207.1 ± 7.4	0.06
7	224.3	157.7 ± 16.5	0.30
8	204.8	229.8 ± 15.3	0.12
9	214.4	183.5 ± 5.1	0.14
10	221.8	493.6 ± 27.7	1.22
11	472.0	357.4 ± 8.5	0.24
12	476.6	321.4 ± 6.6	0.33
13	473.8	327.2 ± 29.2	0.31
14	465.0	298.7 ± 21.1	0.36
15	91.8	128.7 ± 3.9	0.40
16	491.8	435.7 ± 18.8	0.11
17	487.8	375.2 ± 49.4	0.23
18	456.2	328.4 ± 32.5	0.28
19	54.2	-13.4 ± 3.7	1.25
20	201.4	168.8 ± 2.5	0.16
21	281.5	185.1 ± 5.9	0.34
22	461.2	362.2 ± 8.9	0.21
23	474.9	310.1 ± 11.7	0.35
24	481.2	359.4 ± 1.2	0.25

Table S5. Database used to draw contour plot predicting carbon yield when using EI

Number	Metal wt.%	Co wt.%	Mo wt.%	Drying temperature [°C]	Calcination temperature [°C]	Carbon yield [%]
1	1	1	0	228	829	-11.8 ± 6.0
2	70	61	9	205	789	87.2 ± 16.8
3	50	2	48	224	755	-31.6 ± 3.5
4	9	8	1	209	747	20.2 ± 7.8
5	10	1	9	155	729	4.0 ± 15.7
6	63	35	28	92	579	109.8 ± 7.0
7	45	44	1	150	567	233.7 ± 8.2
8	41	32	9	270	539	159.7 ± 57.3
9	22	0	22	145	431	-13.9 ± 12.1
10	60	21	39	233	426	8.9 ± 15.8
11	43	2	41	291	406	-19.8 ± 4.3
12	45	44	1	132	354	170.6 ± 15.3
13	65	54	11	114	311	244.0 ± 20.5
14	61	57	4	123	433	161.0 ± 4.2
15	70	52	18	80	300	107.7 ± 14.8
16	59	48	11	154	300	166.1 ± 8.9
17	42	42	0	183	502	148.8 ± 5.6
18	40	33	7	142	531	164.8 ± 6.8
19	70	51	19	124	300	160.8 ± 16.5
20	58	47	11	108	300	133.6 ± 6.2
21	48	42	6	145	568	212.5 ± 18.1
22	66	59	7	151	300	167.1 ± 6.0
23	45	45	0	129	634	279.1 ± 15.4
24	46	46	0	139	766	499.0 ± 21.1
25	46	46	0	138	832	399.1 ± 24.9
26	46	46	0	164	759	337.0 ± 17.3
27	51	51	0	134	756	295.1 ± 8.1
28	44	44	0	134	767	356.7 ± 12.6
29	47	43	4	136	755	362.0 ± 10.8
30	47	47	0	143	737	446.7 ± 8.9
31	46	46	0	125	766	459.6 ± 15.2
32	49	49	0	91	663	224.9 ± 3.8
33	49	49	0	93	865	262.8 ± 5.7
34	56	56	0	95	813	225.7 ± 4.9
35	52	40	12	93	800	335.7 ± 44.1
36	53	42	11	117	916	324.8 ± 17.6
37	55	41	14	127	779	290.9 ± 14.8

Table S6. Database used to draw contour plot predicting carbon yield when using OKG

Number	Metal wt.%	Co wt.%	Mo wt.%	Drying temperature [°C]	Calcination temperature [°C]	Carbon yield [%]
1	1	1	0	228	829	-11.8 ± 6.0
2	70	61	9	205	789	87.2 ± 16.8
3	50	2	48	224	755	-31.6 ± 3.5
4	9	8	1	209	747	20.2 ± 7.8
5	10	1	9	155	729	4.0 ± 15.7
6	63	35	28	92	579	109.8 ± 7.0
7	45	44	1	150	567	233.7 ± 8.2
8	41	32	9	270	539	159.7 ± 57.3
9	22	0	22	145	431	-13.9 ± 12.1
10	60	21	39	233	426	8.9 ± 15.8
11	43	2	41	291	406	-19.8 ± 4.3
12	45	44	1	132	354	170.6 ± 15.3
13	65	54	11	114	311	244.0 ± 20.5
14	64	59	5	86	400	167.8 ± 8.8
15	61	51	10	174	341	165.9 ± 15.4
16	43	43	0	157	501	177.5 ± 18.2
17	52	44	8	123	479	183.2 ± 12.0
18	39	39	0	119	563	219.6 ± 1.9
19	50	50	0	125	578	207.1 ± 7.4
20	60	46	14	99	308	157.7 ± 16.5
21	43	38	5	134	625	229.8 ± 15.3
22	40	34	6	130	512	183.5 ± 5.1
23	41	41	0	132	753	493.6 ± 27.7
24	41	41	0	154	774	357.4 ± 8.5
25	47	47	0	121	803	321.4 ± 6.6
26	36	36	0	124	758	327.2 ± 29.2
27	41	41	0	125	797	298.7 ± 21.1
28	70	49	21	242	353	128.7 ± 3.9
29	46	46	0	102	730	435.7 ± 18.8
30	44	44	0	142	719	375.2 ± 49.4
31	43	37	6	120	751	328.4 ± 32.5
32	1	1	0	260	626	-13.4 ± 3.7
33	50	50	0	131	587	168.8 ± 2.5
34	48	47	1	96	539	185.1 ± 5.9
35	40	40	0	119	738	362.2 ± 8.9
36	50	50	0	133	757	310.1 ± 11.7
37	38	38	0	138	744	359.4 ± 1.2

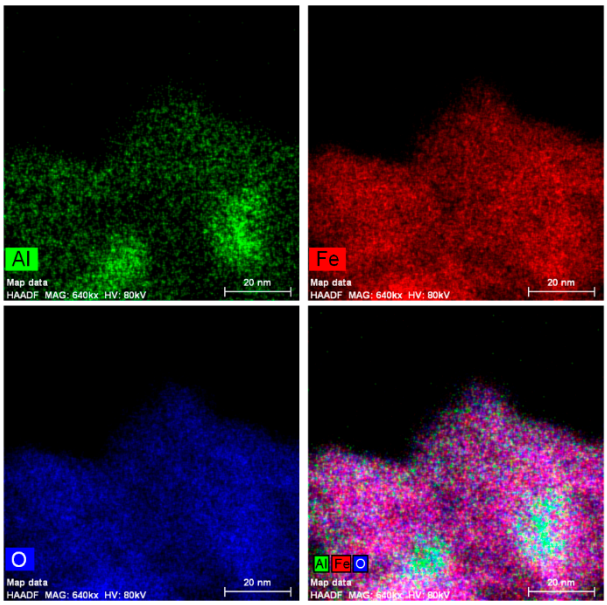

Figure S1. Energy-dispersive X-ray spectroscopy of Fe catalyst distributed on the Al_2O_3.

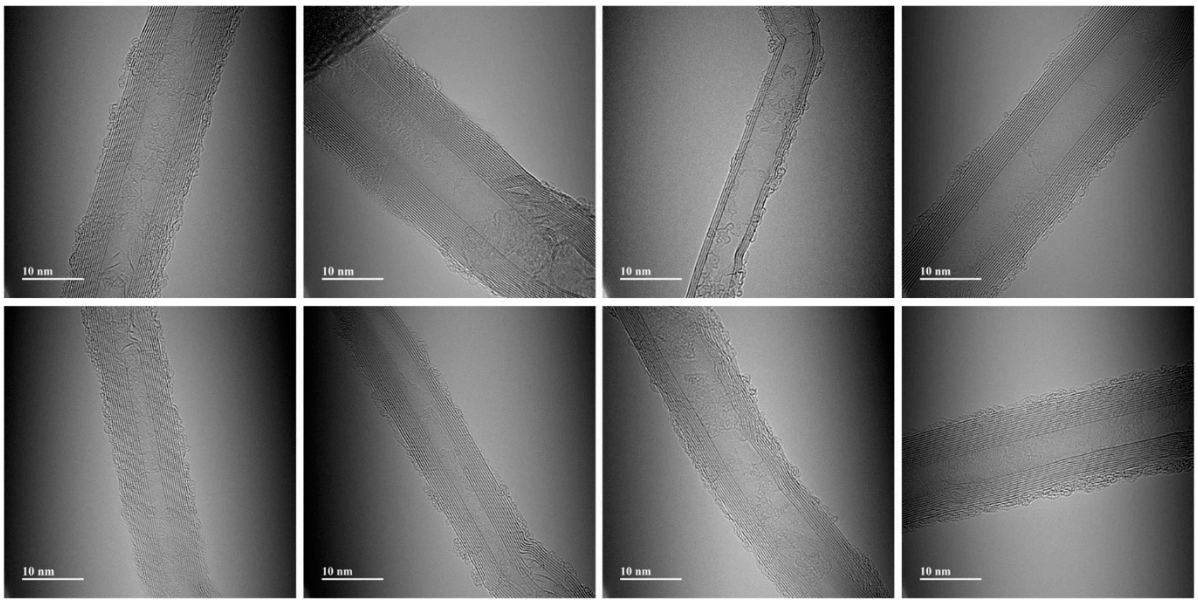

Figure S2. TEM image of as-synthesized CNTs.