

**Table S1:** The selectivity of CO<sub>2</sub> in the different armchair SiC-CNT bundles at 300 K.

(40,40)		(20,20)		(10,10)	
S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)
2.09	1	2.49	1	3.16	1
2.12	3	2.54	3	3.32	3
2.23	5	2.61	5	3.47	5
2.38	7	2.63	7	3.52	7
2.59	9	2.84	9	3.69	9
2.84	10	3.12	10	3.73	10
2.91	20	3.17	20	4.2	20
3.08	30	3.37	30	4.7	30
3.49	40	3.67	40	5.01	40
3.69	50	3.88	50	5.24	50
3.99	60	4.19	60	5.39	60
4.1	70	4.31	70	5.51	70
4.11	80	4.22	80	5.68	80
3.97	90	3.99	90	5.73	90
3.81	100	3.89	100	5.64	100

**Table S2:** The selectivity of CO<sub>2</sub> in the different armchair CNT bundles at 300 K.

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(40,40)		(20,20)		(10,10)	
S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)
1.93	1	2.9	1	4.11	1
1.78	3	2.75	3	4.85	3
1.85	5	2.83	5	5.43	5
1.87	7	2.85	7	5.85	7
2.08	9	3.1	9	6.49	9
2.36	10	3.15	10	6.73	10
2.41	20	3.21	20	7	20
2.61	30	3.43	30	7.32	30
2.91	40	3.59	40	7.53	40
3.18	50	3.87	50	7.67	50
3.49	60	4.07	60	7.77	60
3.61	70	4.17	70	7.72	70
3.52	80	4.01	80	7.39	80
3.29	90	3.84	90	7.04	90
3.04	100	3.58	100	6.55	100

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**Table S3:** The selectivity of CO<sub>2</sub> in the different CNT and SiC-CNT bundles at 300 K.

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CNT (20,0)		CNT (20,20)		SiC- CNT (20,0)		SiC- CNT (20,20)	
S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)
3.6	1	2.9	1	2.88	1	2.49	1
4.41	3	2.75	3	3.02	3	2.54	3
4.91	5	2.83	5	3.16	5	2.61	5
5.29	7	2.85	7	3.2	7	2.63	7
5.79	9	3.1	9	3.36	9	2.84	9
6.07	10	3.15	10	3.42	10	3.12	10
6.39	20	3.21	20	3.79	20	3.17	20
6.69	30	3.43	30	4.29	30	3.37	30
6.88	40	3.59	40	4.58	40	3.67	40
7.01	50	3.87	50	4.78	50	3.88	50
7.1	60	4.07	60	4.94	60	4.19	60
7.07	70	4.17	70	5.05	70	4.31	70
6.75	80	4.01	80	5.21	80	4.22	80
6.43	90	3.84	90	5.19	90	3.99	90
6	100	3.58	100	5.17	100	3.89	100

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**Table S4:** The selectivity of CO<sub>2</sub> in the (20,20) CNT bundles at different temperatures.

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S(CO <sub>2</sub> )	350K		320K		300K		280K	
	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	
2.52	1	2.67	1	2.9	1	3.53	1	
2.23	3	2.33	3	2.75	3	3.57	3	
2.21	5	2.41	5	2.83	5	3.65	5	
2.41	7	2.58	7	2.85	7	3.72	7	
2.98	9	3.08	9	3.1	9	3.52	9	
2.83	10	2.92	10	3.15	10	3.78	10	
2.85	20	2.93	20	3.21	20	3.89	20	
3.12	30	3.2	30	3.43	30	4.06	30	
3.15	40	3.22	40	3.59	40	4.36	40	
3.58	50	3.61	50	3.87	50	4.53	50	
3.61	60	3.66	60	4.07	60	4.88	60	
3.72	70	3.71	70	4.17	70	5.03	70	
3.48	80	3.53	80	4.01	80	4.89	80	
3.44	90	3.52	90	3.84	90	4.56	90	
3.03	100	3.1	100	3.58	100	4.46	100	

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**Table S4 (Continued).** The selectivity of CO<sub>2</sub> in the (20,20) SiC-CNT bundles.

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S(CO <sub>2</sub> )	350K		320K		300K		280K	
	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	S(CO <sub>2</sub> )	P(atm)	
1.94	1	2.05	1	2.49	1	3.13	1	
2	3	2.09	3	2.54	3	3.22	3	
2.03	5	2.13	5	2.61	5	3.35	5	
2.1	7	2.24	7	2.63	7	3.42	7	
2.47	9	2.66	9	2.84	9	3.22	9	
2.79	10	2.86	10	3.12	10	3.58	10	
2.85	20	2.94	20	3.17	20	3.69	20	
3.07	30	3.13	30	3.37	30	3.81	30	
3.39	40	3.43	40	3.67	40	4.11	40	
3.6	50	3.68	50	3.88	50	4.28	50	
3.95	60	4	60	4.19	60	4.58	60	
3.99	70	4.04	70	4.31	70	4.78	70	
3.9	80	3.95	80	4.22	80	4.69	80	
3.78	90	3.82	90	3.99	90	4.36	90	
3.69	100	3.72	100	3.89	100	4.26	100	

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