Supporting Information

Curvature Effect of SiC Nanotubes and Sheet for CO_2 Capture and Reduction

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Table S1. Structure parameters for CO_2 adsorption on SiC sheet and nanotubes. All bond length (r) values are in unit of Å. The corresponding atoms index is shown in Fig. S5.

	$r_{Si1\text{-}O1}$	$r_{C1\text{-}C2}$	$r_{C2\text{-}O1}$		$r_{Si1\text{-}O1}$	$r_{C1\text{-}C2}$	$r_{C2\text{-}O1}$
(3, 0)	1.737	1.524	1.398	(2, 2)	1.723	1.524	1.398
(4, 0)	1.747	1.539	1.382	(3, 3)	1.739	1.544	1.374
(5, 0)	1.754	1.551	1.372	(4, 4)	1.750	1.554	1.363
(6, 0)	1.763	1.561	1.363	(5, 5)	1.756	1.562	1.358
(7, 0)	1.766	1.568	1.358	(6, 6)	1.761	1.567	1.354
(8, 0)	1.771	1.571	1.356	(7, 7)	1.765	1.572	1.351
(9, 0)	1.773	1.577	1.354	(8, 8)	1.768	1.575	1.350
(10, 0)	1.776	1.580	1.351	(9, 9)	1.771	1.578	1.348
(11, 0)	1.777	1.582	1.350	(10, 10)	1.774	1.579	1.347
(12, 0)	1.778	1.584	1.349	SiC layer	1.787	1.595	1.341

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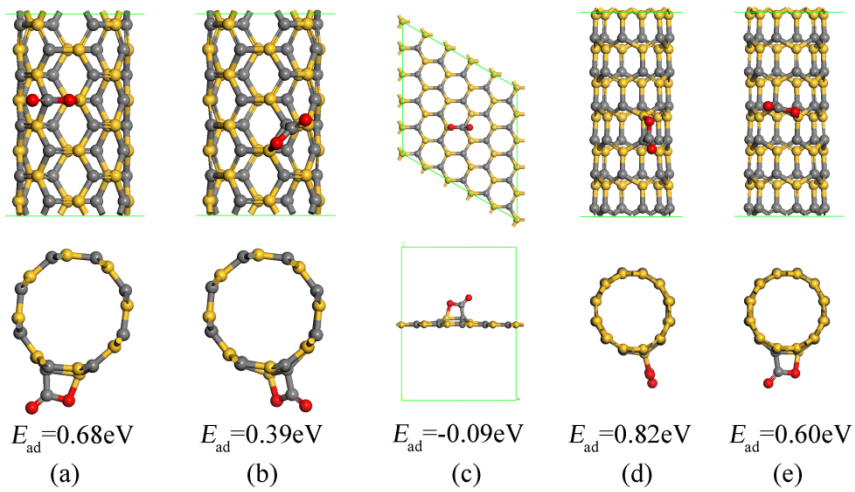

Fig. S1. Optimized adsorption structures of CO_2 adsorbed on (4, 4) armchair SiC nanotubes (a and b),single-layer SiC sheet (c) and (6, 0) zigzag SiC nanotubes (d and e). Gray, gold and red colors denote C, Si and O atoms, respectively.

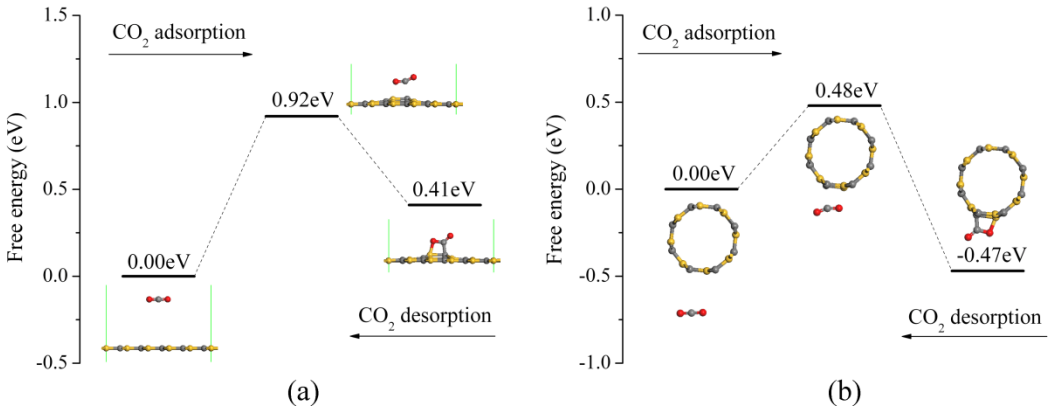

Fig. S2. Free energy diagrams for CO_2 adsorption and desorption processes on single SiC sheet (a) and (4, 4) SiC nanotube (b). Gray, gold and red colors denote C, Si and O atoms, respectively.

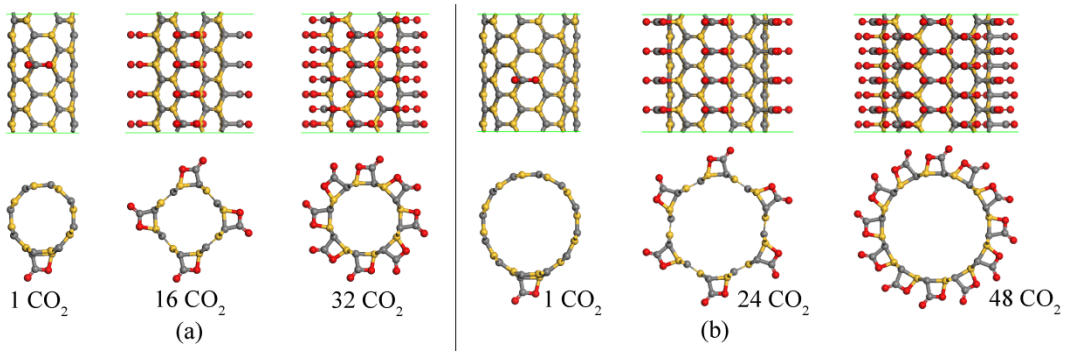

Fig. S3. A schematic plot of CO_2 adsorption on (4, 4) SiC nanotube (a) and (6, 6) SiC nanotube.

Table S2. The average adsorption energies (E_{ad}) for CO_2 molecules adsorbed on (4, 4) and (6, 6) SiC nanotubes. All results are in unit of eV.

	(4, 4)			(6, 6)		
number	1	16	32	1	24	48
E_{ad}	0.68	0.44	0.21	0.35	0.06	−0.28
$(E_{ad})^a$	0.89	0.70	0.51	0.57	0.33	0.04

[a] The energies in parenthesis are performed under the consideration of van der Waals bonding.

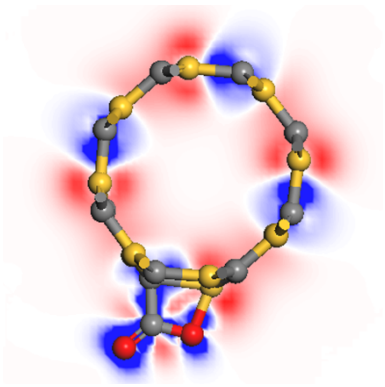

Fig. S4. Electrons density difference of CO_2 adsorbed on (4, 4) SiC nanotubes. The blue region means electronic accumulation, while the red region means electronic loss.

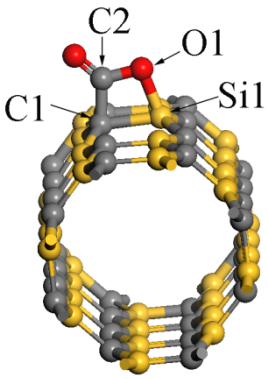

Fig. S5. The corresponding atom index in Tables S1, S3 and S4.

Table S3. Mulliken charge analysis for Si and C atoms bonding with CO_2. Si_{1B} and C_{1B} are the Mulliken charge before CO_2 adsorption. $Si1_A$ and $C1_A$ are the Mulliken charge after CO_2 adsorption. ΔSi1 and ΔC1 are the charge transfer of Si1 and C1 for the CO_2 adsorption process. All results are in unit of *e*. The corresponding atoms index is shown in Fig. S5.

	$Si1_B$	$Si1_A$	ΔSi1	$C1_B$	$C1_A$	ΔC1
(3, 0)	0.897	1.293	0.396	–0.897	–1.088	–0.191
(4, 0)	1.010	1.375	0.365	–1.010	–1.179	–0.169
(5, 0)	1.106	1.420	0.314	–1.106	–1.240	–0.134
(6, 0)	1.158	1.443	0.285	–1.158	–1.277	–0.119
(7, 0)	1.185	1.457	0.272	–1.185	–1.301	–0.116
(8, 0)	1.203	1.464	0.261	–1.203	–1.314	–0.111
(9, 0)	1.214	1.470	0.256	–1.214	–1.324	–0.110
(10, 0)	1.223	1.473	0.250	–1.223	–1.330	–0.107
(11, 0)	1.223	1.474	0.251	–1.223	–1.334	–0.111
(12, 0)	1.234	1.476	0.242	–1.234	–1.337	–0.103
(2, 2)	0.949	1.273	0.324	–0.949	–1.159	–0.210
(3, 3)	1.120	1.393	0.273	–1.120	–1.271	–0.151
(4, 4)	1.180	1.423	0.243	–1.180	–1.302	–0.122
(5, 5)	1.208	1.439	0.231	–1.208	–1.316	–0.108
(6, 6)	1.223	1.446	0.223	–1.223	–1.324	–1.101
(7, 7)	1.231	1.452	0.221	–1.231	–1.328	–0.097
(8, 8)	1.237	1.455	0.218	–1.237	–1.330	–0.093
(9, 9)	1.241	1.457	0.216	–1.241	–1.331	–0.090
(10, 10)	1.245	1.459	0.214	–1.245	–1.332	–0.087
SiC layer	1.261	1.470	0.209	–1.261	–1.328	–0.067

Table S4. Mulliken charge analysis for C and O atoms of CO_2 bonding with SiC. $C2_B$ and $O1_B$ are the Mulliken charges before adsorption. $C2_A$ and $O1_A$ are the Mulliken charges after adsorption. ΔC2 and ΔO1 are the charge transfer for the CO_2 adsorption process. All results are in unit of *e*. The corresponding atoms index is shown in Fig. S5.

	$C2_B$	$C2_A$	ΔC2	$O1_B$	$O1_A$	ΔO1
(3, 0)	0.524	0.568	0.044	–0.349	–0.568	–0.215
(4, 0)	0.529	0.565	0.036	–0.345	–0.565	–0.212
(5, 0)	0.530	0.561	0.031	–0.343	–0.561	–0.210
(6, 0)	0.532	0.553	0.021	–0.340	–0.553	–0.208
(7, 0)	0.532	0.547	0.015	–0.339	–0.547	–0.205
(8, 0)	0.533	0.540	0.007	–0.337	–0.540	–0.205
(9, 0)	0.533	0.536	0.003	–0.337	–0.536	–0.204
(10, 0)	0.534	0.532	–0.002	–0.336	–0.532	–0.203
(11, 0)	0.534	0.530	–0.004	–0.336	–0.50	–0.202
(12, 0)	0.534	0.527	–0.007	–0.336	–0.527	–0.201
(2, 2)	0.521	0.599	0.078	–0.350	–0.574	–0.224
(3, 3)	0.527	0.575	0.048	–0.343	–0.558	–0.215
(4, 4)	0.532	0.558	0.026	–0.343	–0.549	–0.206
(5, 5)	0.530	0.545	0.015	–0.337	–0.544	–0.207
(6, 6)	0.530	0.538	0.008	–0.336	–0.541	–0.205
(7, 7)	0.531	0.533	0.002	–0.335	–0.538	–0.203
(8, 8)	0.532	0.528	–0.004	–0.334	–0.536	–0.202
(9, 9)	0.532	0.524	–0.008	–0.334	–0.535	–0.201
(10, 10)	0.532	0.522	–0.010	–0.333	–0.534	–0.201
SiC layer	0.538	0.505	–0.033	–0.335	–0.526	–0.191