Electronic Supplementary Material (ESI) for New Journal of Chemistry.

"Supporting Information"

Catalytic activity of silicon carbide nanotubes and nanosheets for oxidation of CO: A DFT study

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Figure S1. The optimized structures and electron density difference (EDD) maps (± 0.001 au) of adsorbed singlet O_2 over (6,0) SiCNT. All bond distances are in Å

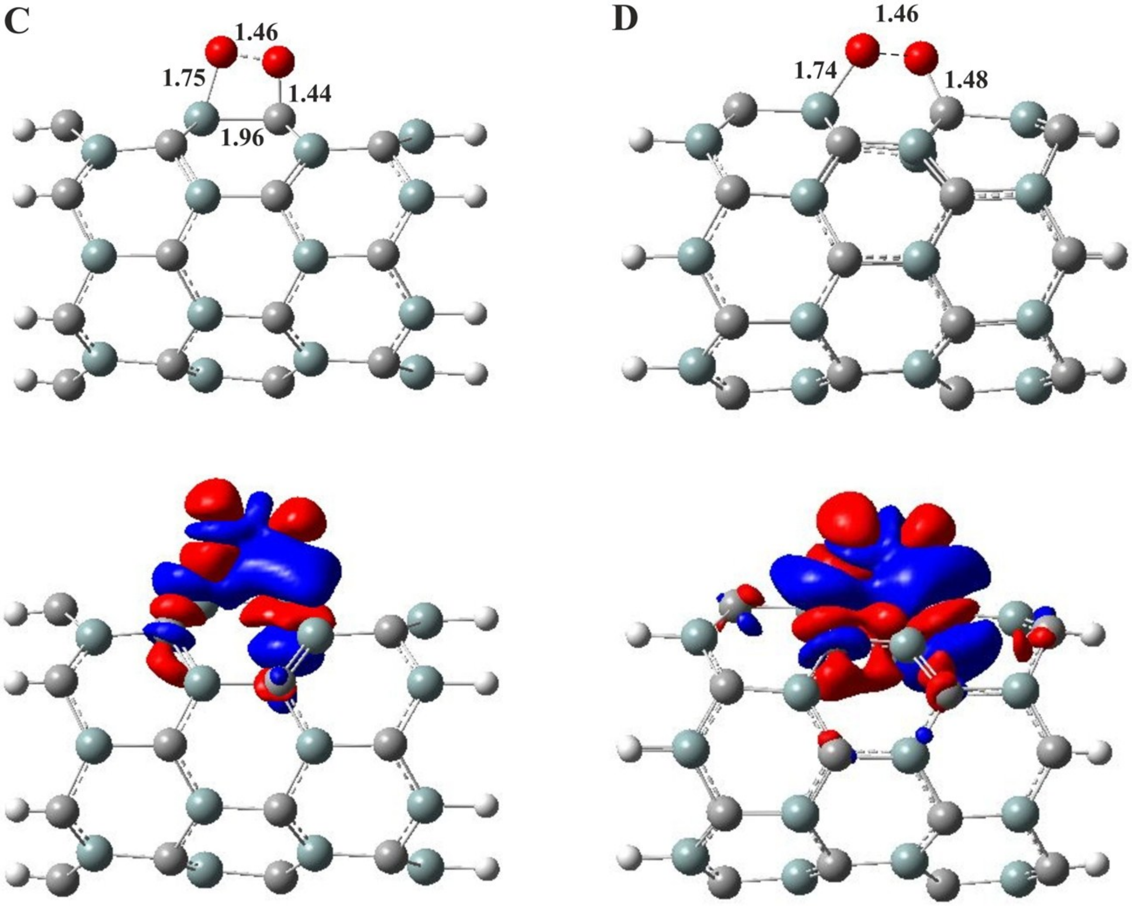


Figure S2. Optimized structures of adsorbed O_2 (triplet) and CO molecule over a long-length (6,0) SiCNT. All bond distances are in Å.

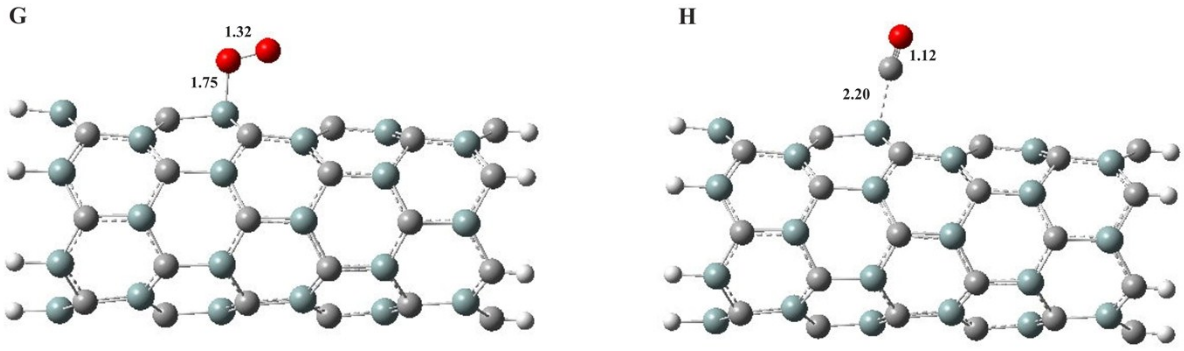


Figure S3. Optimized structures of pristine (5,0) SiCNT and four different adsorption configurations of O_2/CO over a finite-sized (5,0) SiCNT with different spin states. Configurations **I** (**K** and **L**) relate to the triplet (singlet) O_2 molecule. All bond distances are in Å

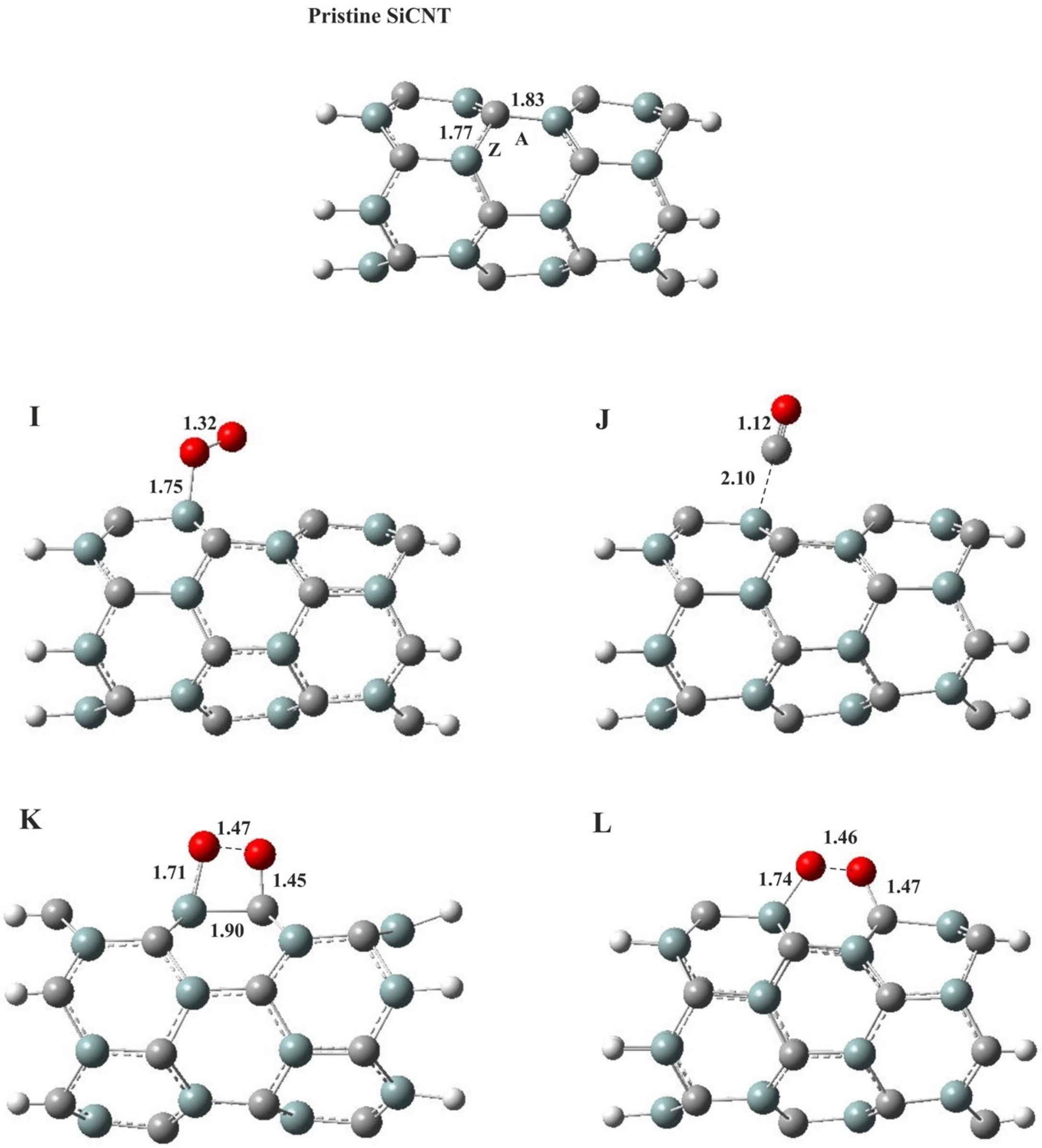
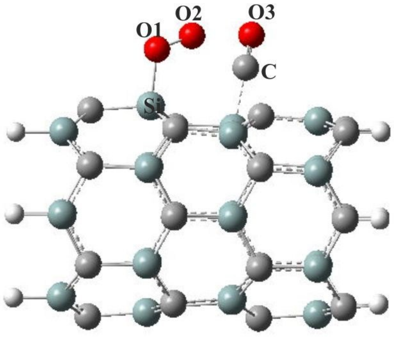
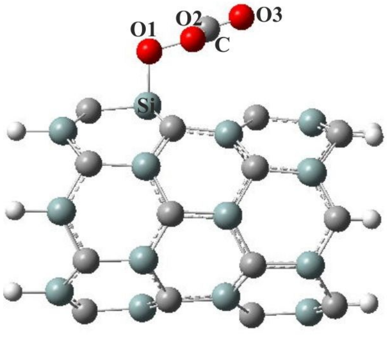


Figure S4. Different calculated initial States (IS) for the CO oxidation reaction. Configurations **M** and **N** relate to the IS-1 while **O** and **P** complexes are obtained for IS-2



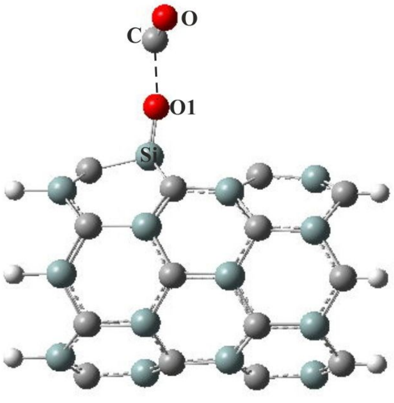
M

r (Si-O1)= 1.77
r (O1-O2)= 1.32
r (O2-C)= 2.72
r (C-O3)=1.26



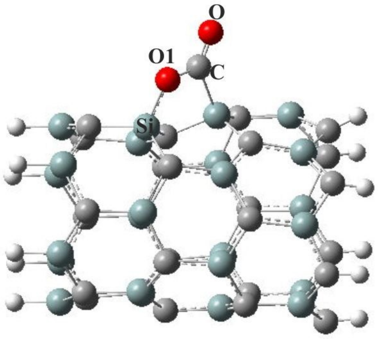
N

r (Si-O1)= 1.73
r (O1-O2)= 1.43
r (O2-C)= 1.34
r (C-O3)= 1.83



O

r (Si-O1)= 1.57
r (O1-C)= 2.43
r(C-O)=1.15



P

r (Si-O1)= 1.96
r (O1-C)= 1.20
r (C-O)= 1.14
r (Si-C)= 1.92

Figure S5. Schematic energy profile corresponding to local configurations along the minimum-energy pathway (MEP) via a) O_2 + CO → O_{ads} + CO_2 and b) O_{ads} + CO → CO_2 reaction mechanisms over (5,0) SiCNT. All energies are in eV.

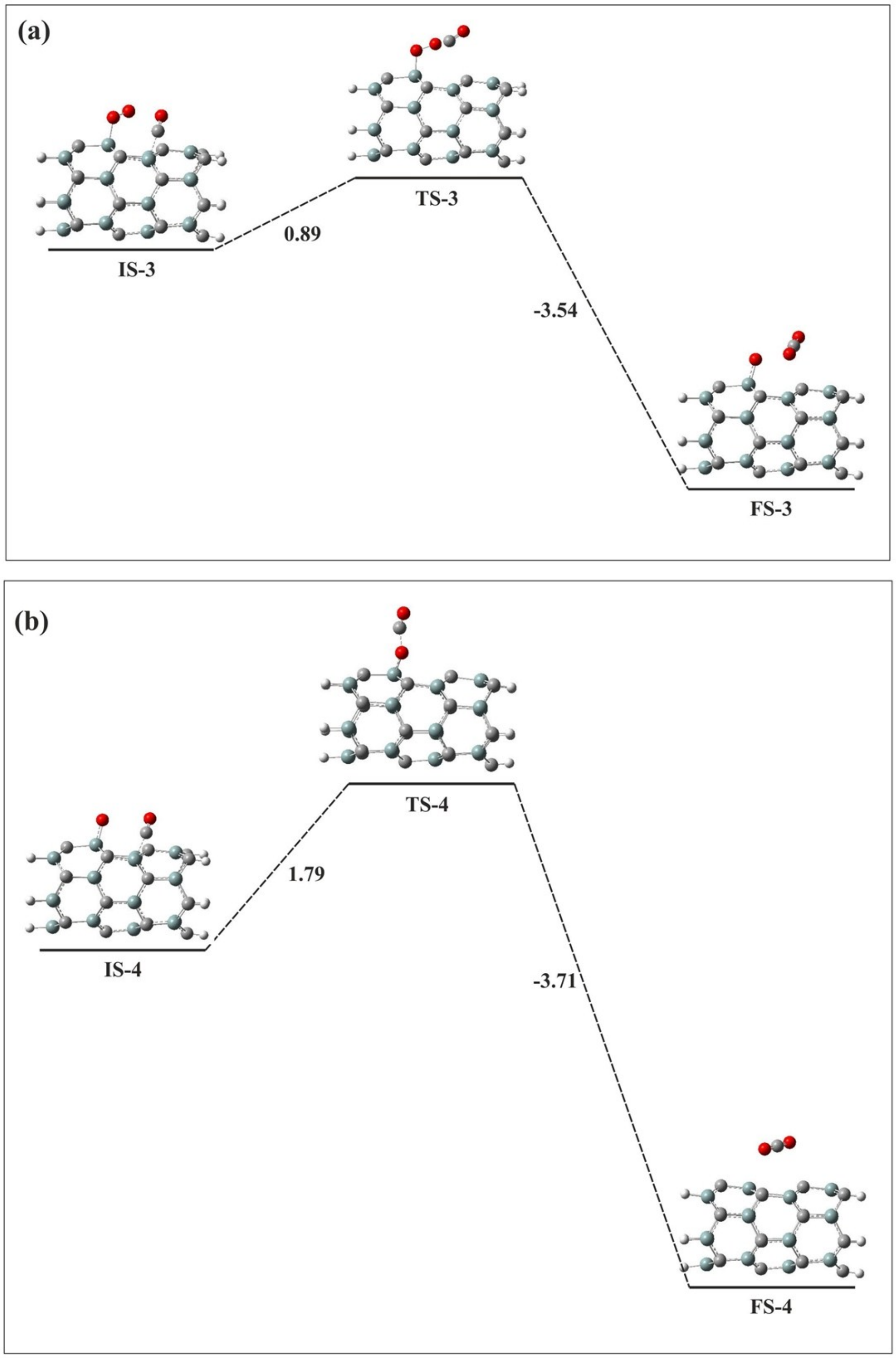
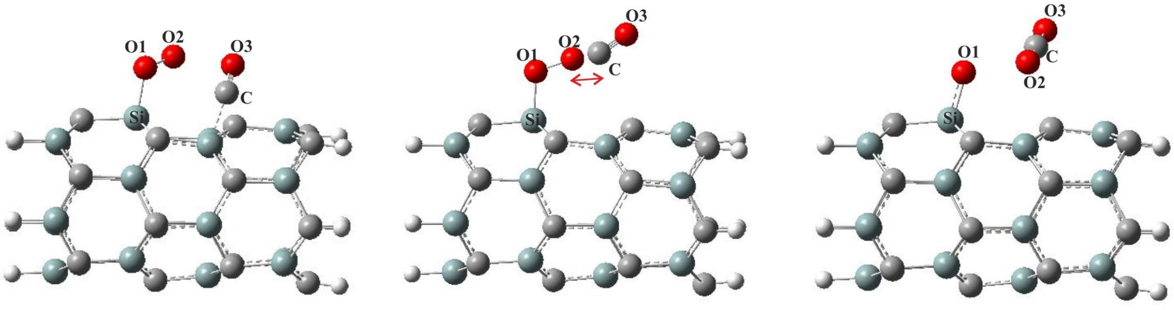


Figure S6. Local configurations of the gas molecules over the (5,0) SiCNT in various states, including the initial state (IS), transition state (TS) and product (P) along the minimum-energy pathway via the O_2 + CO → O_{ads} + CO_2 and O_{ads} + CO → CO_2 routes. All bond distances are in Å. The red arrow shows the imaginary vibration correspond to the TS.



IS-3

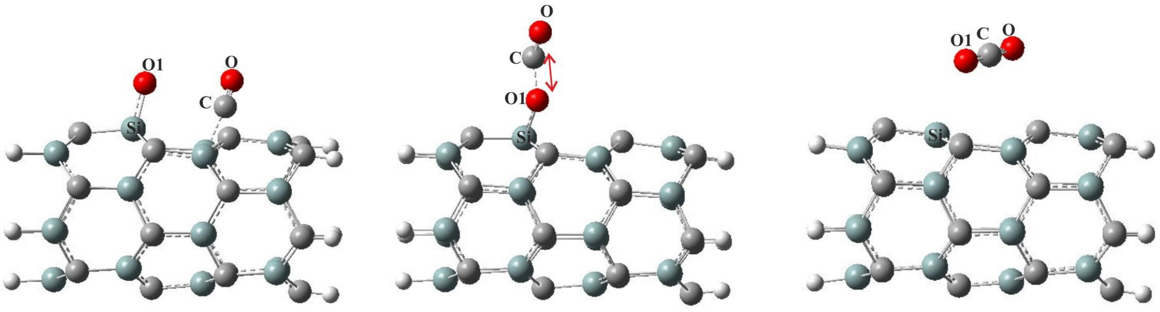
r (Si-O1)= 1.76
r (O1-O2)= 1.32
r (O2-C)= 2.87
r (Si-C)= 2.08
r (C-O3)= 1.12

TS-3

r (Si-O1)= 1.72
r (O1-O2)= 1.37
r (C-O2)= 1.76
r (C-O3)= 1.14

FS-3

r (Si-O1)= 1.67
r (O1-O2)= 2.99
r (O2-C)= 1.17
r (C-O3)= 1.16



IS-4

r (Si-O1)= 1.67
r (O1-C)= 3.88
r (Si-C)= 2.10

TS-4

r (Si-O1)= 1.71
r (O1-C)= 1.56
r (C-O)= 1.15

FS-4

r (Si-O1)= 2.72
r (C-O1)= 1.17
r (C-O)= 1.16
r (Si-C)= 3.37

Figure S7. Schematic energy profile corresponding to local configurations along the minimum-energy pathway (MEP) via a) O_2 + CO → O_{ads} + CO_2 and b) O_{ads} + CO → CO_2 reaction mechanisms over SiCNS. All energies are in eV.

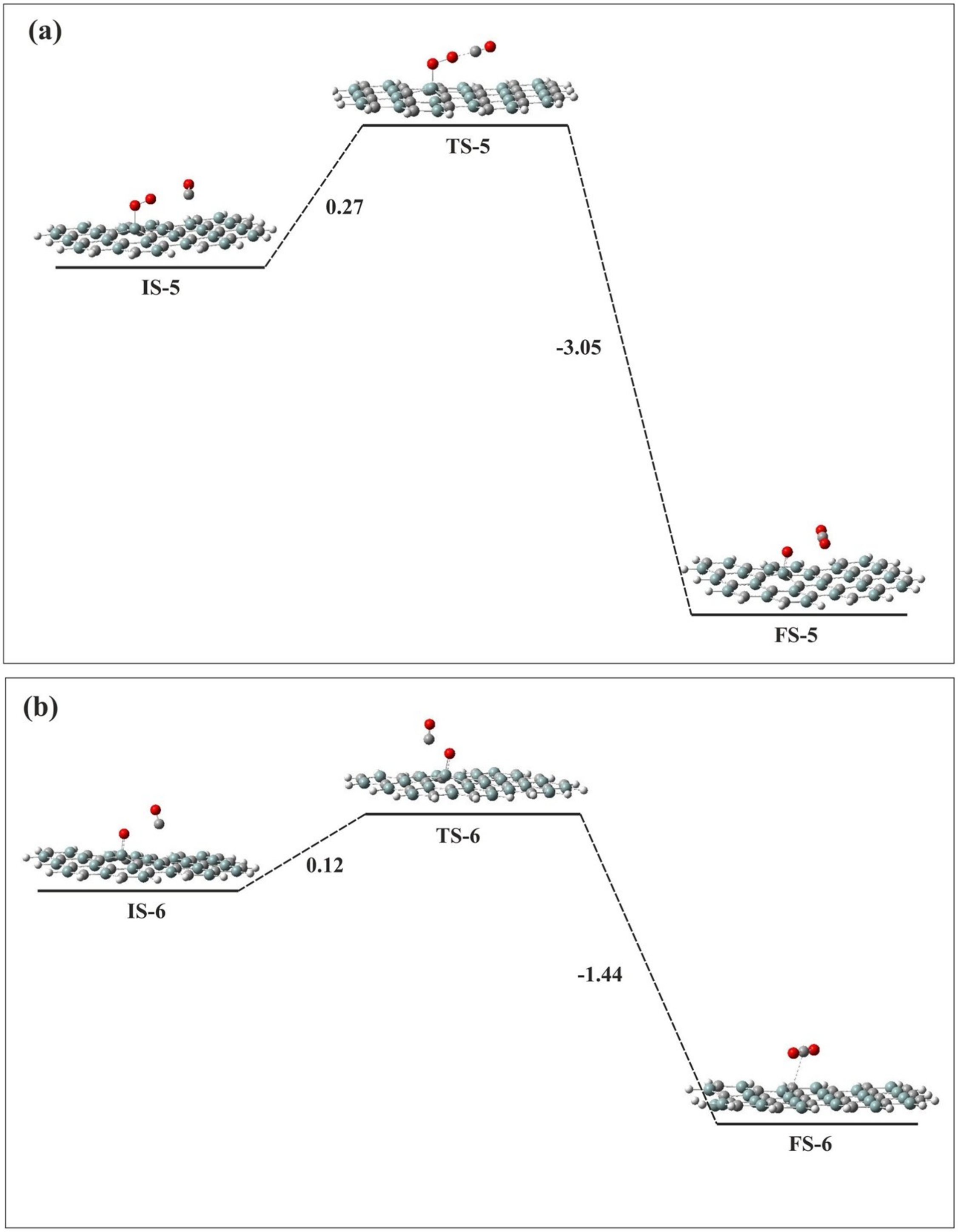
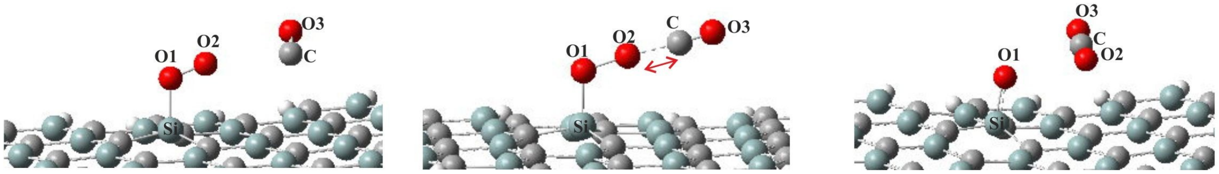


Figure S8. Local configurations of the gas molecules over the SiCNS in various states, including the initial state (IS), transition state (TS) and product (P) along the minimum-energy pathway via the O_2 + CO → O_{ads} + CO_2 and O_{ads} + CO → CO_2 routes. All bond distances are in Å. The red arrow shows the imaginary vibration corresponds to the TS.



IS-5

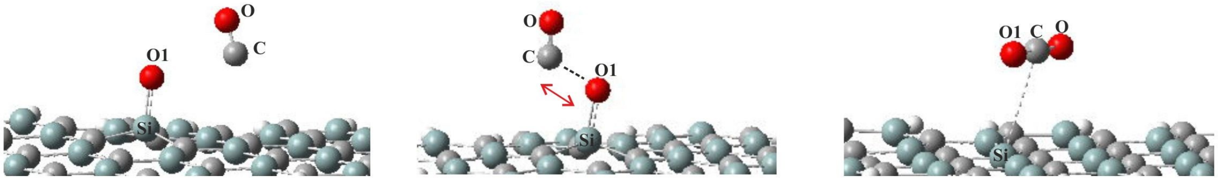
r (Si-O1)= 1.79
r (O1-O2)= 1.32
r (O2-C)= 2.94
r (C-O3)= 1.13

TS-5

r (Si-O1)= 1.78
r (O1-O2)= 1.35
r (C-O2)= 1.76
r (C-O3)= 1.13

FS-5

r (Si-O1)= 1.69
r (O1-O2)= 2.98
r (O2-C)= 1.16
r (C-O3)= 1.16



IS-6

r (Si-O1)= 1.69
r (O1-C)= 2.98
r (C-O)= 1.13

TS-6

r (Si-O1)= 1.70
r (O1-C)= 1.99
r (C-O)= 1.14

FS-6

r (Si-O1)= 3.21
r (C-O1)= 1.16
r (C-O)= 1.16
r (Si-C)= 3.56

Table S1. Calculated binding distances (R), Mulliken charge-transfer (q_{CT}), adsorption energy (E_{ads}), change of Gibbs free energy (ΔG_{298}) and change of enthalpy (ΔH_{298}) of singlet O_2 adsorption over (6,0) SiCNT (large-length (6,0) SiCNT)

configuration	R (Å)	q_{CT} (e)	E_{ads} (eV)	ΔG_{298} (eV)	ΔH_{298} (eV)
C	1.75	-0.65	-2.09	-1.60	-2.06
D	1.74	-0.67	-3.16	-2.64	-3.12
G	1.75	-0.44	-1.39	-	-
H	2.20	0.17	-0.59	-	-

Table S2. Calculated binding distances (R), Mulliken charge-transfer (q_{CT}), adsorption energy (E_{ads}), change of Gibbs free energy (ΔG_{298}) and change of enthalpy (ΔH_{298}) of triplet O_2 (complex **I**), singlet O_2 (complexes **K,L**) and CO (complex **J**) adsorption over (5,0) SiCNT.

configuration	R (Å)	q_{CT} (e)	E_{ads} (eV)	ΔG_{298} (eV)	ΔH_{298} (eV)
I	1.75	-0.42	-1.72	-1.24	-1.70
J	2.11	0.18	-0.51	-0.02	-0.45
K	1.74	0.66	-3.56	-2.98	-3.51
L	1.71	0.63	-3.08	-2.63	-3.10

Table S3. Calculated activation energy (E_{act}), reaction energy (ΔE), change of Gibbs free energy (ΔG_{298}) and change of enthalpy (ΔH_{298}) for different pathways of CO oxidation by O_2 molecule over (5,0) SiCNT

Reaction	E_{act} (eV)	ΔE (eV)	ΔG_{298} (eV)	ΔH_{298} (eV)
IS-3 → FS-3	0.89	-2.65	-2.67	-2.65
IS-4 → FS-4	1.79	-1.92	-1.91	-1.92