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"Supporting Information"

A DFT study on the N_2O reduction by CO molecule over silicon carbide nanotubes and nanosheets

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Figure S1. Optimized structures of pristine, adsorbed N_2O and CO molecule over a (5,0) SiCNT (complexes **I**, **J**) and a long-length (6,0) SiCNT (complexes **K, L**). All bond distances are in Å.

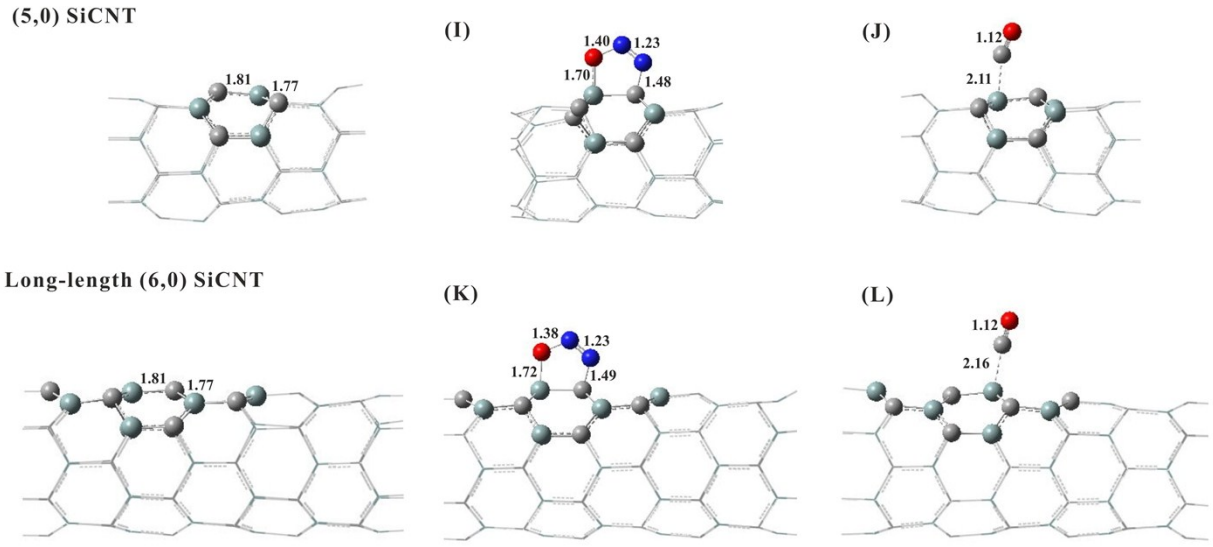
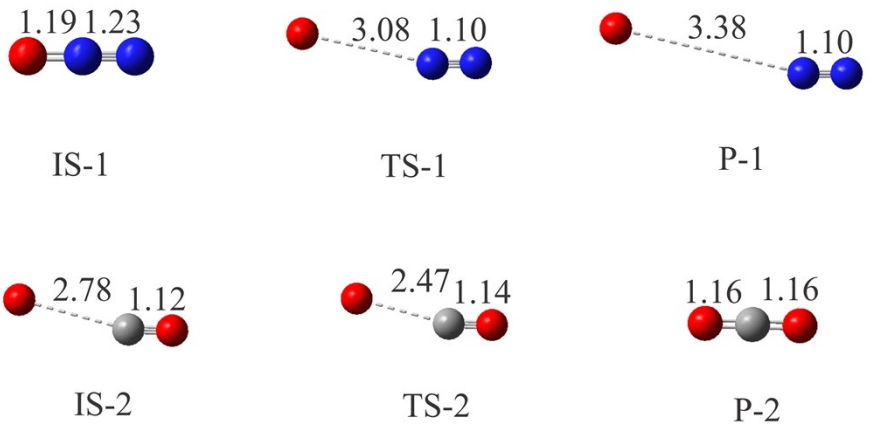


Figure S2. Reaction energy profiles and the corresponding optimized structures (at the M062X/6-31G* level) of the stationary points for the direct reduction of N_2O by CO. All energy values and distances are in eV and Å, respectively.



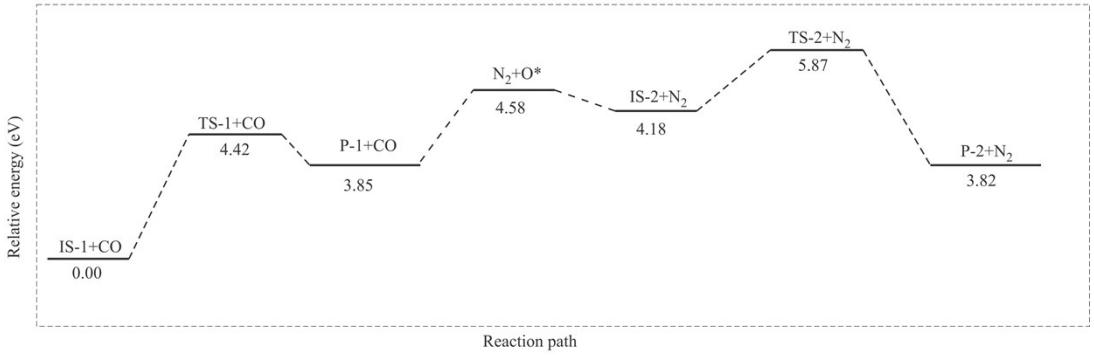


Figure S3. Reaction energy profiles and the corresponding optimized structures of the stationary points for the reduction of N_2O by CO over the (5,0) SiCNT. All energy values and distances are in eV and Å, respectively.

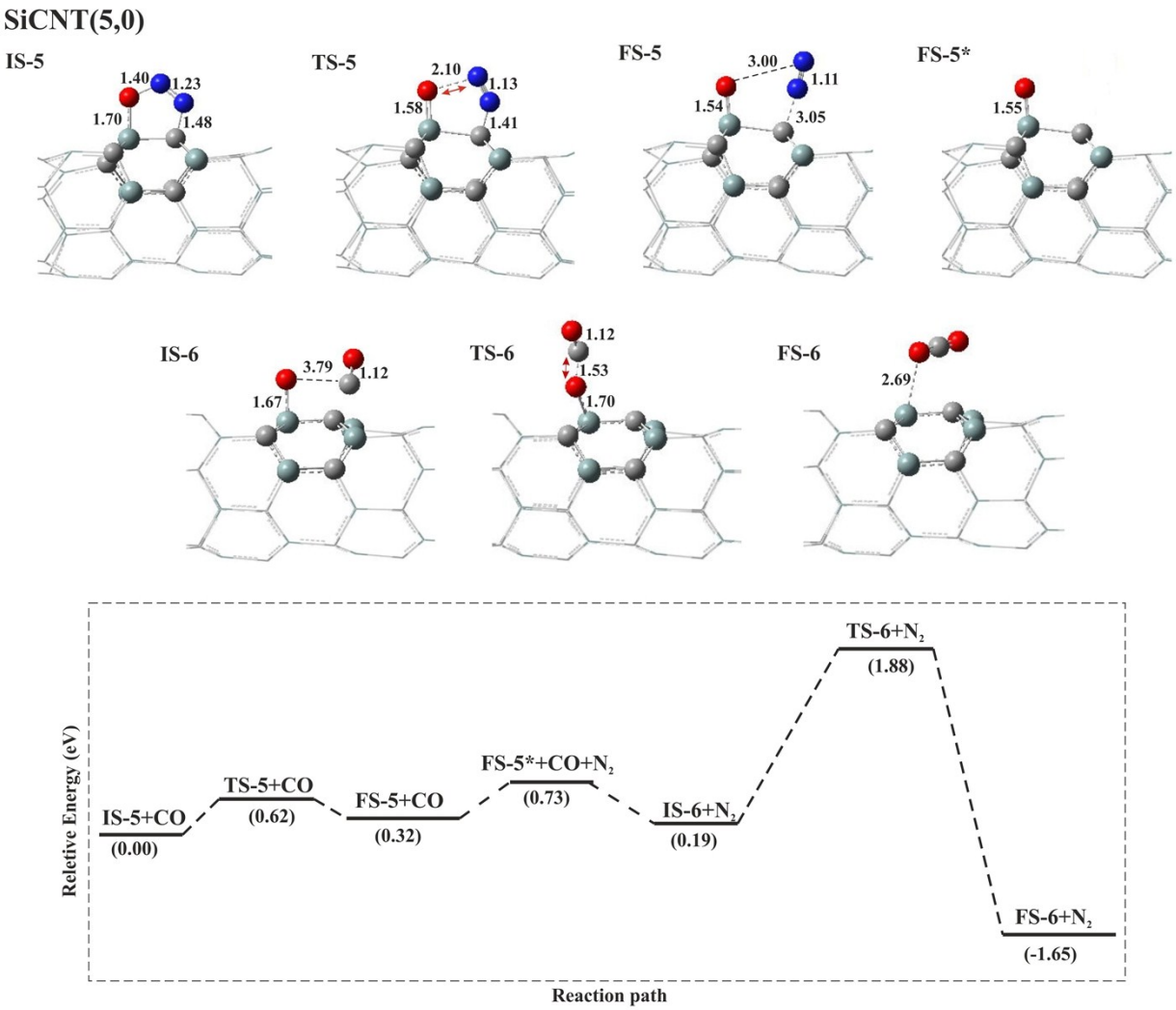


Table S1. Calculated binding distances (R), adsorption energies (E_{ads}), Mulliken ($q_{CT,M}$) and Hirshfeld ($q_{CT,H}$) charge-transfer values of adsorbed N_2O and CO molecules over the (5,0) SiCNT (complexes **E** and **F**) and long-length (6,0) SiCNT (complexes **G** and **H**)

configuration	R (Å)	E_{ads} (eV)	$q_{CT,M}$ (e)	$q_{CT,H}$ (e)
(5,0) SiCNT				
E	1.70	-0.86	0.54	0.32
F	2.11	-0.48	0.17	0.12
Long-length (6,0) SiCNT				
G	1.72	-0.69	0.55	0.30
H	2.16	-0.47	0.16	0.10

Table S2. Calculated activation energy (E_{act}) and reaction energy (ΔE) for different pathways of reduction of N_2O by CO molecule over (5,0) SiCNT

Reaction	E_{act} (eV)	ΔE (eV)
(5,0) SiCNT		
IS-5 → FS-5	0.62	0.32
IS-6 → FS-6	1.69	-1.84