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"Supporting Information"

Can Si-embedded boron nitride nanotubes act as a favorable metal-free catalyst for CO oxidation by N_2O?

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Figure S1. The optimized structures of the pristine long-length (6,0) BNNT along with the Si-doped configurations. All bond distances are in Å

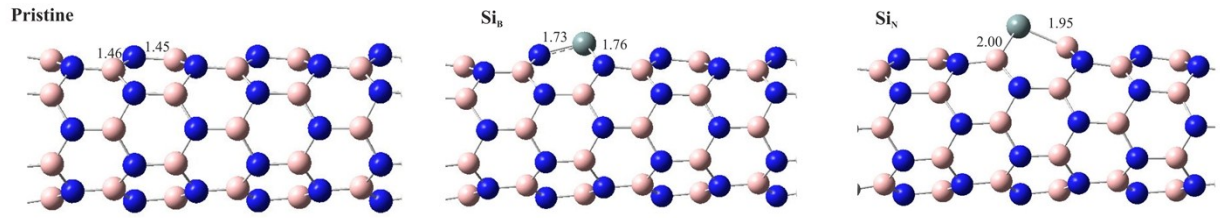

Figure S2. Optimized structures of adsorbed N_2O/CO molecules over a long-length (6,0) BNNT. All bond distances are in Å.

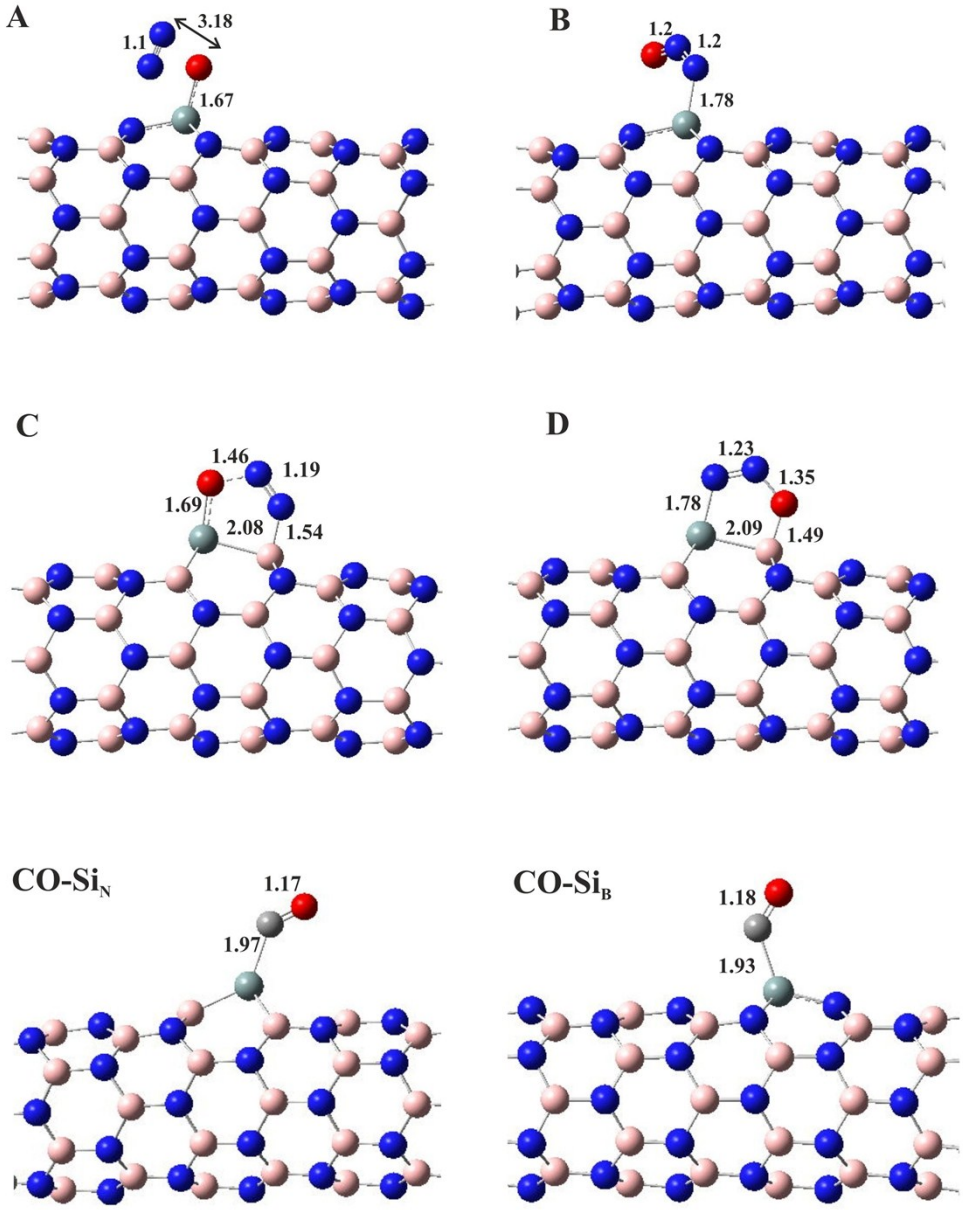

Figure S3. Local configurations of the gas molecules over the long-length (6,0) BNNT in various states, including the initial state (IS), transition state (TS) and final state (FS) along the minimum-energy pathway via the $N_2O \rightarrow O^* + N_2$ and $O^* + CO \rightarrow CO_2$ routes. All bond distances are in Å.

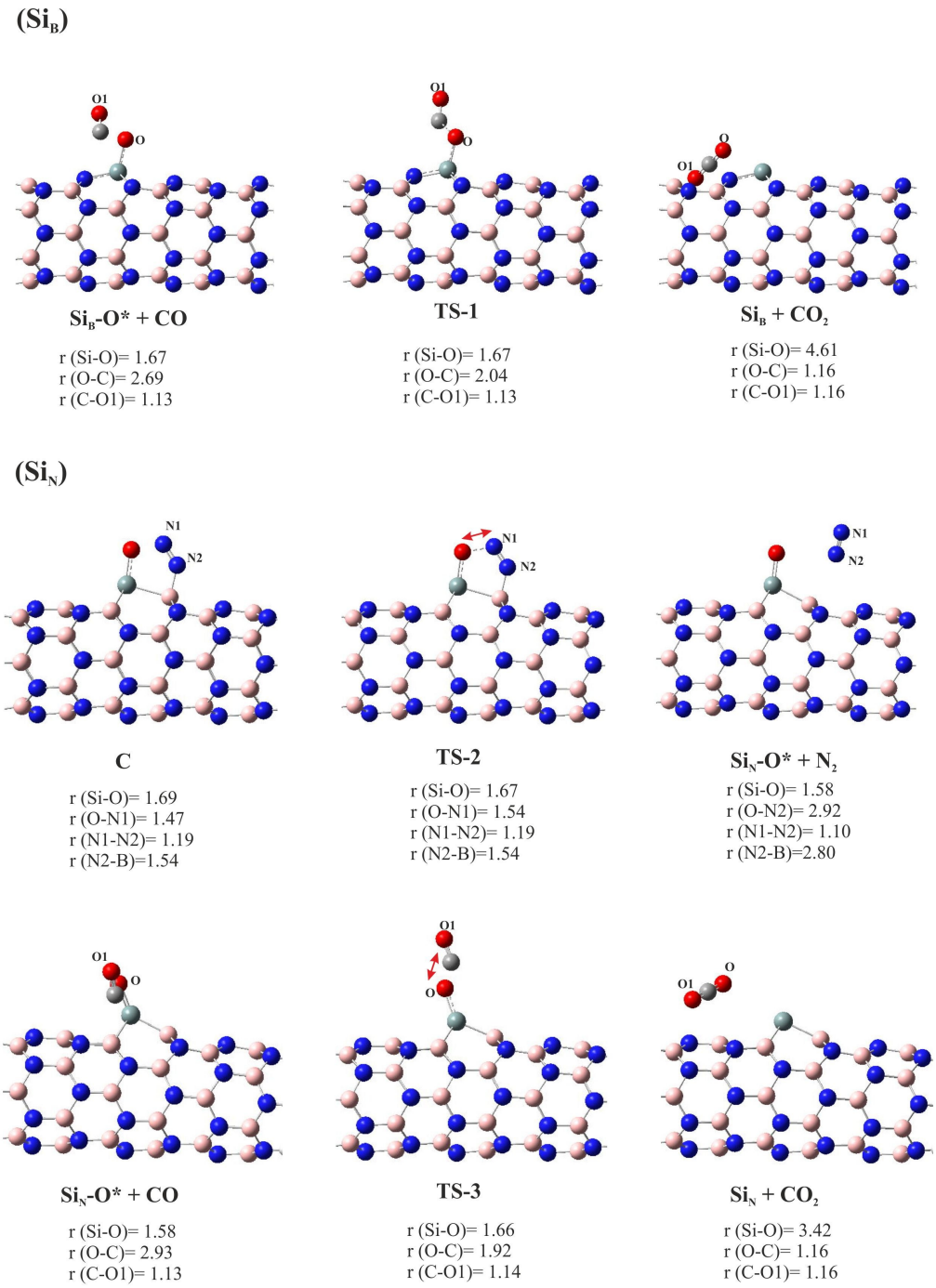

Table S1. Calculated binding distances (R) and adsorption energies (E_{ads}) of the N_2O/CO adsorption over the long-length (6,0) BNNT

configuration	R (Å)	E_{ads} (kcal/mol)
N_2O-Si_B		
A	1.67	-79.21
B	1.78	-26.93
N_2O-Si_N		
C	1.69	-28.89
D	1.78	-20.32
CO-Si_B	1.93	-5.01
CO-Si_N	1.97	-4.10