

Supplementary Information for:

**CO oxidation on metal-free nitrogen-doped
carbon nanotubes and the related
structure-reactivity relationships**

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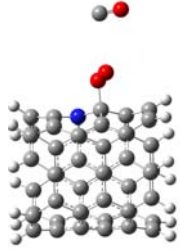
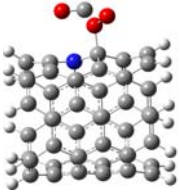
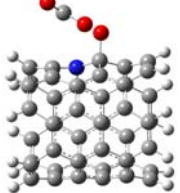
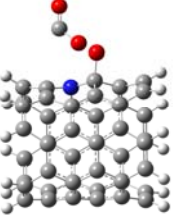

Index

1. The optimized structures of different states in pathway B, C, E and F
2. The IRC analysis results
3. The adsorbing potential energy curve

1. The optimized structures of different states in pathway B, C, E and

F

Table S1. The optimized structures of different states in pathway B and C.

Bond Length in Å	Rea-B	TS1-B	Int-B	TS2-B	Pro-B
					
C _{NCNT} -O _{oxygen}	1.533	1.497	1.453	1.452	1.223
O _{oxygen} -O _{oxygen}	1.316	1.384	1.478	1.484	3.050
C _{CO} -O _{oxygen}	3.067	1.735	1.343	1.399	1.170
C _{CO} -O _{CO}	1.139	1.157	1.193	1.182	1.169


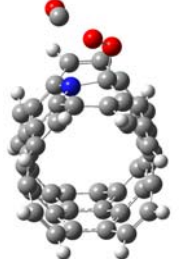
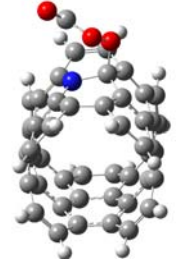
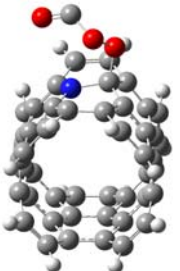
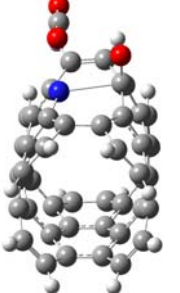

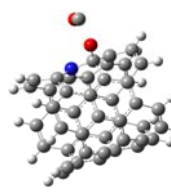
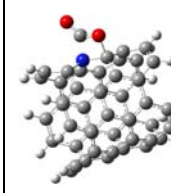
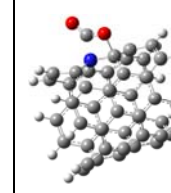
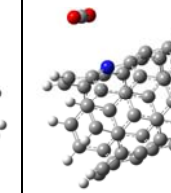
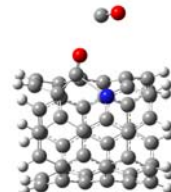
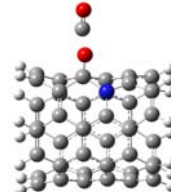
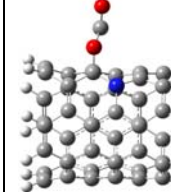
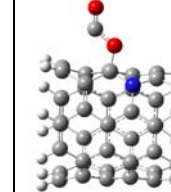
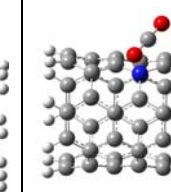
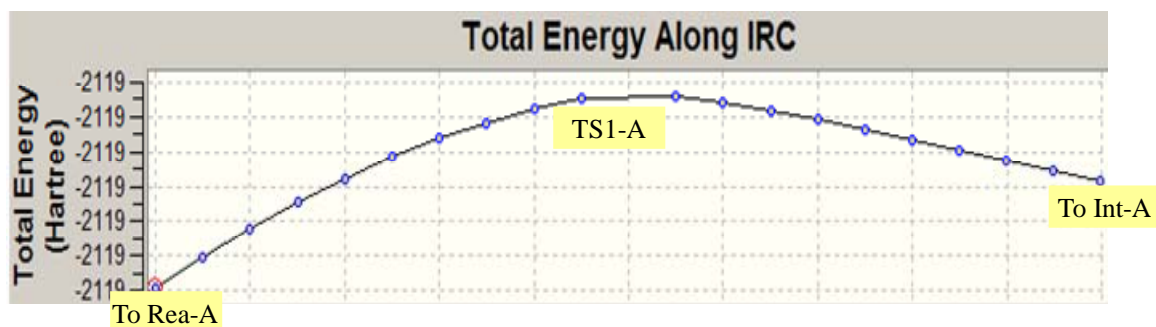
Bond Length in Å	Rea-C	TS1-C	Int-C	TS2-C	Pro-C
					
C _{NCNT} -O _{oxygen}	1.533	1.467	1.459	1.459	1.231
O _{oxygen} -O _{oxygen}	1.316	1.397	1.478	1.504	3.093
C _{CO} -O _{oxygen}	3.050	1.743	1.343	1.389	1.170
C _{CO} -O _{CO}	1.139	1.159	1.192	1.185	1.169

Table S2. The optimized structures of different states in pathway E and F.

Bond Length in Å	Rea-E	TS1-E	Int-E	TS2-E	Pro-E
					
$C_{\text{NCNT}}-O_{\text{oxygen}}$	1.220	1.375	1.534	1.609	3.985
$C_{\text{CO}}-O_{\text{oxygen}}$	2.953	1.866	1.329	1.311	1.169
$C_{\text{CO}}-O_{\text{CO}}$	1.139	1.159	1.183	1.185	1.169
Bond Length in Å	Rea-F	TS1-F	Int-F	TS2-F	Pro-F
					
$C_{\text{NCNT}}-O_{\text{oxygen}}$	1.221	1.350	1.478	1.491	3.985
$C_{\text{CO}}-O_{\text{oxygen}}$	2.951	1.847	1.339	1.336	1.169
$C_{\text{CO}}-O_{\text{CO}}$	1.139	1.161	1.192	1.193	1.169

2. The IRC analysis results.



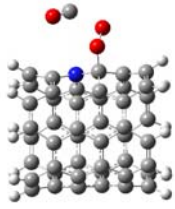
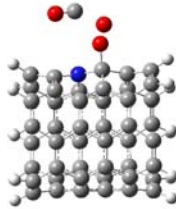
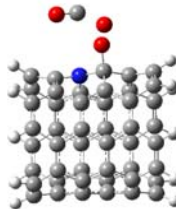
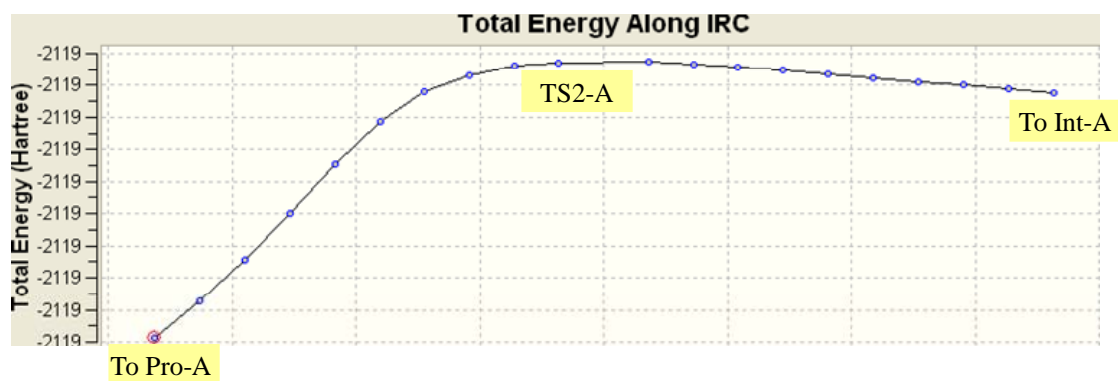
Bond Length	To Rea-A	TS1-A	To Int-A
			
C _{NCNT} -O _{oxygen}	1.487	1.466	1.452
O _{oxygen} -O _{oxygen}	1.341	1.390	1.461
C _{CO} -O _{oxygen}	2.014	1.770	1.525
C _{CO} -O _{CO}	1.145	1.155	1.178

Fig. S1. The IRC analysis result of TS1-A



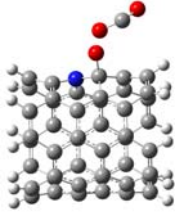
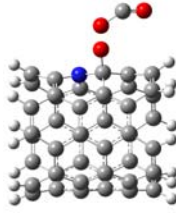
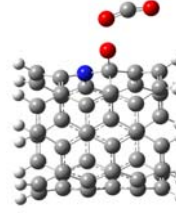
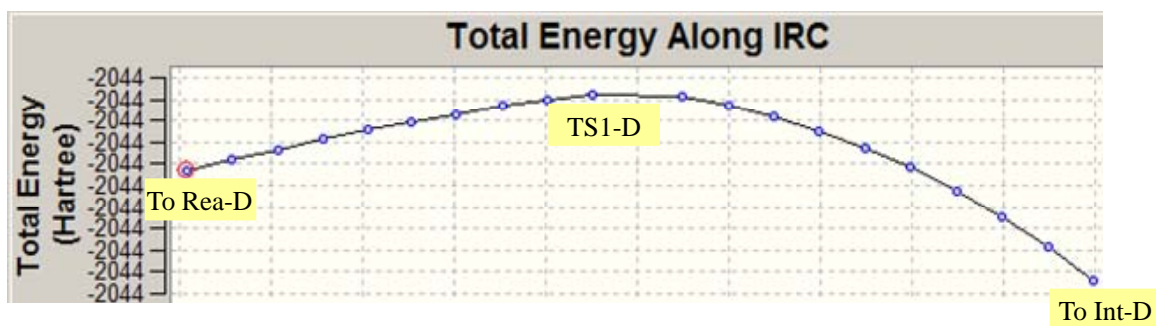
Bond Length	To Int-A	TS2-A	To Pro-A
			
C _{NCNT} -O _{oxygen}	1.437	1.434	1.352
O _{oxygen} -O _{oxygen}	1.500	1.518	1.887
C _{CO} -O _{oxygen}	1.348	1.382	1.168
C _{CO} -O _{CO}	1.190	1.187	1.170
∠COO	102.8	105.3	106.2
∠OCOO	150.7	98.5	60.4

Fig. S2. The IRC analysis result of TS2-A



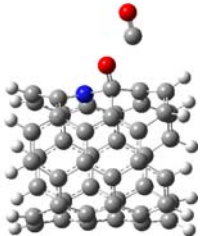
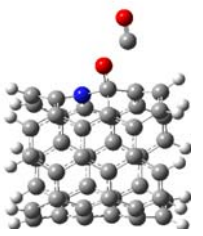
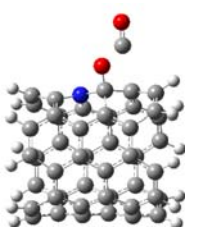
Bond Length	To Rea-D	TS1-D	To Int-D
			
C _{NCNT} -O _{oxygen}	1.285	1.311	1.354
C _{CO} -O _{oxygen}	2.109	1.944	1.751
C _{CO} -O _{CO}	1.149	1.158	1.171

Fig. S3. The IRC analysis result of TS1-D

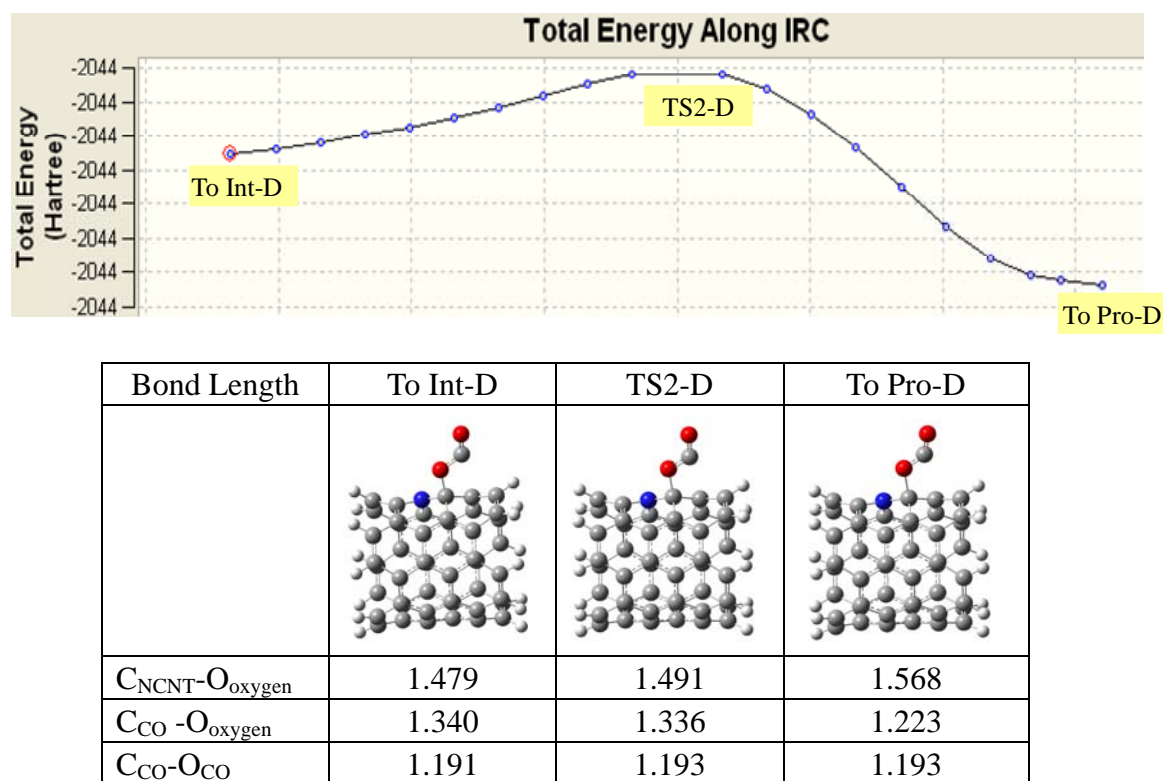


Fig. S4. The IRC analysis result of TS2-D

3. The adsorbing potential energy curve.

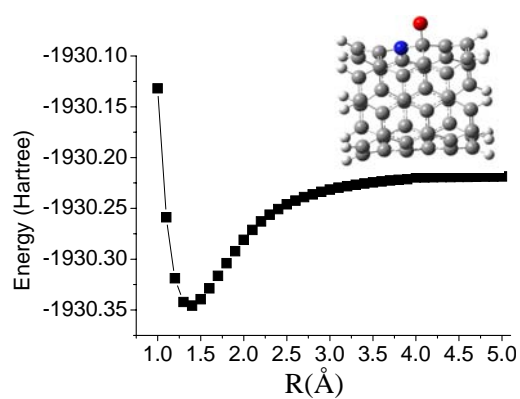


Fig. S5. The adsorbing potential energy curve of NCNT(4,4)-8.0...O.