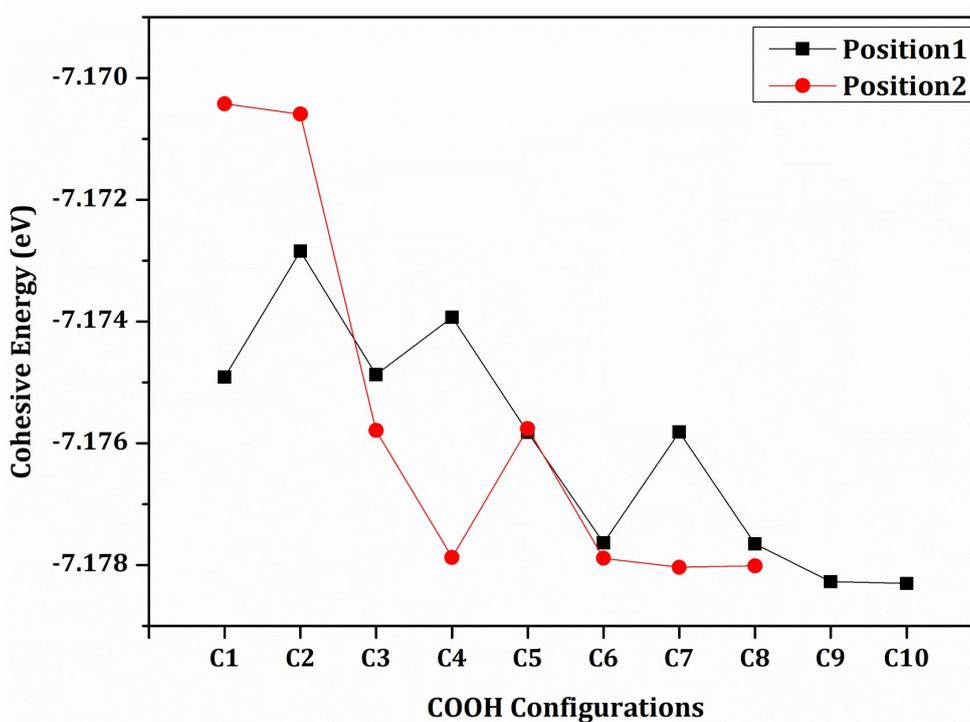


Supplementary Information

Computational Investigation of Carboxyl-Functionalized Hydrogen-Substituted Graphdiyne for Tracing and Trapping Nitrogen and its oxides

Rohith Ramasamy and Rajadurai Vijay Solomon*

Department of Chemistry, Madras Christian College (Autonomous),
[Affiliated to University of Madras], Chennai – 600 059, Tamil Nadu, India
vjsolo@gmail.com



SIF1. Computed cohesive energy (E_{coh}) of COOH configurations at positions 1 and 2

SIT1. Selected Bond Parameters of COOH Configurations at Positions 1 and 2

		Bond parameters												
				C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	
Bond length (Å)	Position - 1													
	Initial	COOH1	C - C	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540
			C - O	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360
			O - H	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960
			C - O	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230
		COOH2	C - C	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540
			C - O	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360
			O - H	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960
			C - O	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230
	Relaxed	COOH1	C - C	1.487	1.487	1.490	1.487	1.500	1.500	1.490	1.500	1.501	1.501	1.501
			C - O	1.362	1.364	1.358	1.364	1.358	1.358	1.362	1.358	1.356	1.356	1.356
			O - H	0.979	0.979	0.979	0.979	0.981	0.981	0.979	0.981	0.981	0.981	0.981
			C - O	1.223	1.221	1.222	1.222	1.215	1.214	1.222	1.214	1.215	1.215	1.215
		COOH2	C - C	1.489	1.487	1.487	1.486	1.489	1.500	1.501	1.500	1.501	1.501	1.501
			C - O	1.358	1.364	1.362	1.364	1.362	1.358	1.358	1.358	1.356	1.356	1.356
			O - H	0.979	0.979	0.979	0.980	0.979	0.981	0.981	0.981	0.981	0.981	0.981
			C - O	1.222	1.221	1.223	1.222	1.222	1.214	1.215	1.214	1.215	1.215	1.215
	Position - 2													
	Initial	COOH1	C - C	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	-	-
			C - O	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	-	-
			O - H	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	-	-
			C - O	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	-	-
		COOH2	C - C	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	1.540	-	-
			C - O	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	1.360	-	-
			O - H	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	0.960	-	-
			C - O	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	1.230	-	-
	Relaxed	COOH1	C - C	1.494	1.494	1.501	1.501	1.490	1.501	1.501	1.501	1.501	-	-
			C - O	1.362	1.361	1.356	1.357	1.362	1.358	1.357	1.357	1.357	-	-
		O - H	0.980	0.980	0.981	0.981	0.979	0.981	0.981	0.981	0.981	-	-	
		C - O	1.221	1.222	1.215	1.215	1.222	1.214	1.215	1.215	1.215	-	-	
COOH2		C - C	1.494	1.494	1.490	1.500	1.501	1.500	1.500	1.500	1.500	-	-	
		C - O	1.362	1.361	1.362	1.358	1.356	1.357	1.357	1.357	1.357	-	-	

			O - H	0.980	0.980	0.979	0.981	0.981	0.981	0.981	0.981	-	-	
			C - O	1.221	1.221	1.222	1.214	1.214	1.215	1.215	1.215	-	-	
Bond Angle (°)	Position - 1													
	Initial	COOH1	C - O - H	109.50	109.50	109.50	109.50	109.51	109.51	109.50	109.51	109.51	109.51	109.51
			C - C - O	120.00	120.00	120.00	120.00	119.99	119.99	120.00	120.01	120.01	120.01	119.99
		COOH2	C - O - H	109.51	109.50	109.50	109.51	109.51	109.49	109.49	109.49	109.49	109.49	109.49
			C - C - O	120.00	120.00	120.00	120.00	120.00	120.00	120.00	120.00	120.00	120.00	120.00
	Relaxed	COOH1	C - O - H	105.02	104.69	105.98	104.29	106.59	106.61	104.85	106.63	106.73	106.76	
			C - C - O	124.33	124.21	124.45	124.72	124.01	123.84	124.62	123.64	123.86	123.99	
		COOH2	C - O - H	105.94	104.71	105.01	104.26	104.91	106.63	106.57	106.64	106.75	106.75	
			C - C - O	124.39	124.21	124.40	124.70	124.52	123.75	123.94	123.74	123.92	123.93	
	Position - 2													
	Initial	COOH1	C - O - H	109.50	109.50	109.49	109.49	109.51	109.51	109.51	109.50	-	-	
			C - C - O	120.00	120.00	120.01	120.01	120.00	120.00	120.00	120.01	-	-	
		COOH2	C - O - H	109.50	109.50	109.50	109.51	109.51	109.51	109.51	109.51	-	-	
			C - C - O	120.00	120.00	120.00	120.00	120.00	120.00	120.00	120.00	-	-	
	Relaxed	COOH1	C - O - H	104.36	104.31	106.63	106.63	104.77	106.64	106.73	106.72	-	-	
			C - C - O	124.60	124.49	123.57	123.85	124.33	123.88	123.86	123.83	-	-	
COOH2		C - O - H	104.37	104.49	104.75	106.63	106.60	106.62	106.73	106.70	-	-		
		C - C - O	124.61	124.48	124.36	123.88	123.57	123.87	123.86	123.85	-	-		
Dihedral Angle (°)	Position - 1													
	Initial	COOH1	C - C - O - H	180.00	180.00	180.00	180.00	180.00	180.00	180.00	179.99	179.99	180.00	
			C - C - C - O	180.00	180.00	179.90	179.90	89.90	89.90	179.84	90.11	90.11	90.08	
		COOH2	C - C - O - H	180.00	180.00	180.00	180.00	180.00	180.00	180.00	180.00	180.00	180.00	
			C - C - C - O	179.99	179.94	179.94	179.82	179.82	89.86	89.86	89.83	89.92	89.83	
	Relaxed	COOH1	C - C - O - H	179.94	179.96	179.98	179.87	179.83	179.98	179.00	179.98	179.21	179.21	
			C - C - C - O	179.97	179.88	179.82	179.79	88.83	88.19	179.55	88.15	88.81	88.84	
		COOH2	C - C - O - H	179.87	179.99	180.00	179.95	178.94	179.75	179.91	179.73	179.31	179.30	
			C - C - C - O	179.89	179.88	179.96	179.83	179.57	88.06	88.68	88.16	88.97	88.90	
	Position - 2													
	Initial	COOH1	C - C - O - H	180.00	180.00	180.00	180.00	180.00	180.00	180.00	180.00	-	-	
			C - C - C - O	179.99	179.99	89.93	89.93	179.98	89.97	89.97	89.96	-	-	
		COOH2	C - C - O - H	180.00	180.00	179.99	180.00	180.00	179.99	180.00	179.99	-	-	
			C - C - C - O	180.00	179.89	179.95	90.01	90.01	90.02	90.00	90.02	-	-	
	Relaxed	COOH1	C - C - O - H	179.97	179.95	179.63	179.75	179.83	179.77	179.79	179.76	-	-	
			C - C - C - O	179.84	179.81	88.24	88.42	179.92	88.54	88.52	88.40	-	-	

		COOH2	C - C - O - H	179.97	179.95	179.88	179.67	179.66	179.68	179.69	179.69	-	-
			C - C - C - O	179.94	179.80	179.91	88.36	88.32	88.21	88.29	88.14	-	-

SIT2. Optimized atomic coordinates of the COOH-HsGDY supercell (2 × 2 × 1)

C	-1.1936640000	10.1558440000	2.3689560000
H	-2.1386560000	10.6958100000	2.3662800000
C	-1.2061610000	8.7457430000	2.3768470000
C	-2.4396310000	8.0393620000	2.3773760000
C	-3.5037580000	7.4240020000	2.3690170000
C	0.0201730000	10.8740220000	2.3634620000
C	0.0199550000	12.2967130000	2.3497360000
C	0.0226540000	13.5264780000	2.3392650000
C	1.2364040000	10.1592220000	2.3687780000
C	0.0253400000	8.0462540000	2.3809320000
C	7.0243150000	5.4210260000	2.3206920000
C	1.2552010000	8.7491630000	2.3768630000
H	2.1792160000	10.7027340000	2.3632270000
C	5.7965650000	6.1398100000	2.3261990000
C	2.4916230000	8.0457310000	2.3735560000
C	4.7322000000	6.7555130000	2.3425200000
C	3.5574330000	7.4324440000	2.3583900000
C	7.0317280000	4.0042260000	2.3252540000
C	8.2542400000	6.1106340000	2.3187130000
H	8.2532780000	7.1987650000	2.3177560000
C	9.4813170000	5.4148750000	2.3252450000

C	8.2536010000	3.2871720000	2.3247020000
C	9.4675970000	4.0045560000	2.3252810000
C	10.7124230000	6.1264260000	2.3384340000
C	8.2584530000	1.8647030000	2.3259070000
H	10.4085450000	3.4573740000	2.3278240000
C	11.7762480000	6.7425700000	2.3543040000
C	8.2553120000	0.6351230000	2.3303420000
C	0.0338450000	6.5468840000	2.3216680000
O	0.0432370000	5.9080710000	1.2882160000
O	0.0359680000	5.9929500000	3.5597190000
H	0.0545240000	5.0203890000	3.4344060000
C	5.7304650000	3.2605780000	2.4020430000
O	5.1824720000	2.9586060000	3.4434640000
O	5.2390450000	2.9719680000	1.1712830000
H	4.3901240000	2.5005500000	1.3093420000
C	-9.4193140000	24.4030880000	2.3689560000
H	-10.3643060000	24.9430540000	2.3662800000
C	-9.4318110000	22.9929870000	2.3768470000
C	-10.6652810000	22.2866050000	2.3773760000
C	-11.7294080000	21.6712450000	2.3690170000
C	-8.2054770000	25.1212660000	2.3634620000
C	-8.2056950000	26.5439570000	2.3497360000
C	-8.2029960000	27.7737220000	2.3392650000
C	-6.9892460000	24.4064660000	2.3687780000

C	-8.2003100000	22.2934970000	2.3809320000
C	-1.2013350000	19.6682690000	2.3206920000
C	-6.9704490000	22.9964060000	2.3768630000
H	-6.0464340000	24.9499780000	2.3632270000
C	-2.4290850000	20.3870540000	2.3261990000
C	-5.7340270000	22.2929750000	2.3735560000
C	-3.4934500000	21.0027570000	2.3425200000
C	-4.6682170000	21.6796880000	2.3583900000
C	-1.1939220000	18.2514690000	2.3252540000
C	0.0285900000	20.3578780000	2.3187130000
H	0.0276280000	21.4460090000	2.3177560000
C	1.2556670000	19.6621190000	2.3252450000
C	0.0279510000	17.5344160000	2.3247020000
C	1.2419470000	18.2518000000	2.3252810000
C	2.4867730000	20.3736700000	2.3384340000
C	0.0328030000	16.1119470000	2.3259070000
H	2.1828950000	17.7046180000	2.3278240000
C	3.5505980000	20.9898140000	2.3543040000
C	0.0296620000	14.8823670000	2.3303420000
C	-8.1918050000	20.7941280000	2.3216680000
O	-8.1824130000	20.1553150000	1.2882160000
O	-8.1896820000	20.2401940000	3.5597190000
H	-8.1711260000	19.2676320000	3.4344060000
C	-2.4951850000	17.5078220000	2.4020430000

O	-3.0431780000	17.2058490000	3.4434640000
O	-2.9866050000	17.2192120000	1.1712830000
H	-3.8355260000	16.7477940000	1.3093420000
C	15.2576360000	10.1558440000	2.3689560000
H	14.3126440000	10.6958100000	2.3662800000
C	15.2451390000	8.7457430000	2.3768470000
C	14.0116690000	8.0393620000	2.3773760000
C	12.9475420000	7.4240020000	2.3690170000
C	16.4714730000	10.8740220000	2.3634620000
C	16.4712550000	12.2967130000	2.3497360000
C	16.4739540000	13.5264780000	2.3392650000
C	17.6877040000	10.1592220000	2.3687780000
C	16.4766400000	8.0462540000	2.3809320000
C	23.4756150000	5.4210260000	2.3206920000
C	17.7065010000	8.7491630000	2.3768630000
H	18.6305160000	10.7027340000	2.3632270000
C	22.2478650000	6.1398100000	2.3261990000
C	18.9429230000	8.0457310000	2.3735560000
C	21.1835000000	6.7555130000	2.3425200000
C	20.0087330000	7.4324440000	2.3583900000
C	23.4830280000	4.0042260000	2.3252540000
C	24.7055400000	6.1106340000	2.3187130000
H	24.7045780000	7.1987650000	2.3177560000
C	25.9326170000	5.4148750000	2.3252450000

C	24.7049010000	3.2871720000	2.3247020000
C	25.9188970000	4.0045560000	2.3252810000
C	27.1637230000	6.1264260000	2.3384340000
C	24.7097530000	1.8647030000	2.3259070000
H	26.8598450000	3.4573740000	2.3278240000
C	28.2275480000	6.7425700000	2.3543040000
C	24.7066120000	0.6351230000	2.3303420000
C	16.4851450000	6.5468840000	2.3216680000
O	16.4945370000	5.9080710000	1.2882160000
O	16.4872680000	5.9929500000	3.5597190000
H	16.5058240000	5.0203890000	3.4344060000
C	22.1817650000	3.2605780000	2.4020430000
O	21.6337720000	2.9586060000	3.4434640000
O	21.6903450000	2.9719680000	1.1712830000
H	20.8414240000	2.5005500000	1.3093420000
C	7.0319860000	24.4030880000	2.3689560000
H	6.0869940000	24.9430540000	2.3662800000
C	7.0194890000	22.9929870000	2.3768470000
C	5.7860190000	22.2866050000	2.3773760000
C	4.7218920000	21.6712450000	2.3690170000
C	8.2458230000	25.1212660000	2.3634620000
C	8.2456050000	26.5439570000	2.3497360000
C	8.2483040000	27.7737220000	2.3392650000
C	9.4620540000	24.4064660000	2.3687780000

C	8.2509900000	22.2934970000	2.3809320000
C	15.2499650000	19.6682690000	2.3206920000
C	9.4808510000	22.9964060000	2.3768630000
H	10.4048660000	24.9499780000	2.3632270000
C	14.0222150000	20.3870540000	2.3261990000
C	10.7172730000	22.2929750000	2.3735560000
C	12.9578500000	21.0027570000	2.3425200000
C	11.7830830000	21.6796880000	2.3583900000
C	15.2573780000	18.2514690000	2.3252540000
C	16.4798900000	20.3578780000	2.3187130000
H	16.4789280000	21.4460090000	2.3177560000
C	17.7069670000	19.6621190000	2.3252450000
C	16.4792510000	17.5344160000	2.3247020000
C	17.6932470000	18.2518000000	2.3252810000
C	18.9380730000	20.3736700000	2.3384340000
C	16.4841030000	16.1119470000	2.3259070000
H	18.6341950000	17.7046180000	2.3278240000
C	20.0018980000	20.9898140000	2.3543040000
C	16.4809620000	14.8823670000	2.3303420000
C	8.2594950000	20.7941280000	2.3216680000
O	8.2688870000	20.1553150000	1.2882160000
O	8.2616180000	20.2401940000	3.5597190000
H	8.2801740000	19.2676320000	3.4344060000
C	13.9561150000	17.5078220000	2.4020430000

O	13.4081220000	17.2058490000	3.4434640000
O	13.4646950000	17.2192120000	1.1712830000
H	12.6157740000	16.7477940000	1.3093420000

SIT3. Optimized atomic coordinates of the most stable COOH-HsGDY + nitrogen and its oxides adsorbed systems

COOH-HsGDY + N ₂ adsorbed system				COOH-HsGDY + NO adsorbed system			
C	-1.1941350076	10.1504083126	2.3335827301	C	-1.1862929742	10.1578930838	2.3477028172
H	-2.1406901454	10.6872838792	2.3276375861	H	-2.1333410427	10.6939557994	2.3467206955
C	-1.2045159448	8.7400612218	2.3477932591	C	-1.1951546682	8.7477644951	2.3597639741
C	-2.4368371033	8.0313876062	2.3517801834	C	-2.4273709693	8.0379761291	2.3670989552
C	-3.5003861038	7.4150489007	2.3526331944	C	-3.4926997033	7.4237946752	2.3704129864
C	0.0183125469	10.8718757297	2.3315064997	C	0.0248872076	10.8809627807	2.3418226781
C	0.0155981451	12.2953299671	2.3304122340	C	0.0193276034	12.3033854967	2.3406492656
C	0.0179417451	13.5257959798	2.3345631035	C	0.0210513742	13.5332687207	2.3436821742
C	1.2353082813	10.1577599309	2.3348910187	C	1.2436092324	10.1704216678	2.3402724408
C	0.0278540204	8.0425449553	2.3596015617	C	0.0389874791	8.0534035918	2.3622722011
C	7.0276705693	5.4250989324	2.3470526080	C	7.0193901009	5.4147360165	2.3586195884
C	1.2561058570	8.7477452828	2.3480442623	C	1.2659208556	8.7611107899	2.3480493192
H	2.1783802939	10.7008701393	2.3303252293	H	2.1854306333	10.7161293289	2.3365180903
C	5.7998522675	6.1431432520	2.3440245050	C	5.7990906872	6.1432919701	2.3511153966
C	2.4935233298	8.0464664247	2.3508555936	C	2.5028412794	8.0606878964	2.3489708676
C	4.7349442865	6.7579155300	2.3450721710	C	4.7376771005	6.7634031668	2.3486356455
C	3.5597712230	7.4340569263	2.3480677362	C	3.5666707693	7.4446190784	2.3494947557
C	7.0346186612	4.0082150707	2.3417400121	C	7.0112075501	3.9984177171	2.3425662317
C	8.2571800824	6.1146416263	2.3544684579	C	8.2553019097	6.0918539138	2.3770835317
H	8.2552193444	7.2030125588	2.3565640822	H	8.2653652063	7.1801652431	2.3857198039
C	9.4836599541	5.4177953654	2.3562183741	C	9.4749308136	5.3831863874	2.3799450671
C	8.2552999625	3.2891743512	2.3450749512	C	8.2246570639	3.2686677371	2.3540591545
C	9.4692900192	4.0069397779	2.3526116767	C	9.4461516602	3.9730940514	2.3740363945
C	10.7153672536	6.1277177745	2.3573634826	C	10.7116737145	6.0843313372	2.3792678713
C	8.2574730792	1.8661752578	2.3410465497	C	8.2159488607	1.8467836077	2.3456979744

H	10.4103444215	3.4601826799	2.3535410879	H	10.3804912130	3.4147242926	2.3780616540
C	11.7796976425	6.7432846384	2.3540944734	C	11.7758000836	6.7006183631	2.3705443669
C	8.2493398511	0.6360926078	2.3391056029	C	8.2110593553	0.6172001269	2.3428514452
C	0.0360112174	6.5420503376	2.3336552900	C	0.0539611829	6.5532735203	2.3347727579
O	0.0488275775	5.8776783479	1.3167584703	O	0.1196972421	5.8894449138	1.3195648190
O	0.0309271650	6.0201906603	3.5860534943	O	-0.0098396849	6.0305727220	3.5852501788
H	0.0450734881	5.0444816808	3.4875690188	H	0.0152032263	5.0549511100	3.4871697918
C	5.7310638392	3.2672632374	2.3912864209	C	5.7010441040	3.2671989191	2.3649640144
O	5.1604821821	2.9640042506	3.4200875365	O	5.0911770833	2.9933358505	3.3793932748
O	5.2658308991	2.9849781856	1.1488187277	O	5.2802484274	2.9523390264	1.1143626833
H	4.4117825480	2.5171008241	1.2650003085	H	4.4227313176	2.4864422306	1.2133575599
C	-9.4184949726	24.3994762880	2.3342339982	C	-9.4360957912	24.3734931256	2.3417493523
H	-10.3649903847	24.9364751267	2.3293331454	H	-10.3867869092	24.9032719395	2.3386189394
C	-9.4290044139	22.9892811154	2.3454988353	C	-9.4373670530	22.9632007979	2.3548847933
C	-10.6619555916	22.2818938383	2.3454675952	C	-10.6648175588	22.2455220699	2.3560389406
C	-11.7271097780	21.6682471261	2.3459130294	C	-11.7242235695	21.6214814110	2.3544720752
C	-8.2060911929	25.1206220806	2.3328409338	C	-8.2283845143	25.1028133590	2.3368926217
C	-8.2094340560	26.5438898134	2.3312078392	C	-8.2399553308	26.5257087882	2.3336312292
C	-8.2079598779	27.7741957866	2.3350714061	C	-8.2415207780	27.7557703951	2.3378703028
C	-6.9889667670	24.4068070291	2.3354660118	C	-7.0061186468	24.3974460426	2.3398997395
C	-8.1966714586	22.2918861669	2.3585196823	C	-8.2001976626	22.2739473932	2.3646056422
C	-1.1962886325	19.6741978236	2.3464429359	C	-1.1981243426	19.6760906381	2.3567473404
C	-6.9682164478	22.9968501063	2.3478018927	C	-6.9762085585	22.9875036413	2.3523955992
H	-6.0460695501	24.9502730837	2.3308128860	H	-6.0672848787	24.9482652031	2.3380847177
C	-2.4236142245	20.3931746918	2.3435907181	C	-2.4261475050	20.3937501107	2.3510658612
C	-5.7311360600	22.2948062932	2.3504851172	C	-5.7353139743	22.2923397613	2.3537339903
C	-3.4899666700	21.0058666336	2.3459898462	C	-3.4922622624	21.0067192984	2.3480971463
C	-4.6652903425	21.6812619230	2.3489512065	C	-4.6682499429	21.6809927904	2.3506093991
C	-1.1924840137	18.2571403242	2.3420757333	C	-1.1926282625	18.2594839575	2.3382508890
C	0.0346694899	20.3617417587	2.3536506868	C	0.0315471389	20.3652481445	2.3741744636
H	0.0342060289	21.4501685744	2.3567970090	H	0.0298632322	21.4536648633	2.3817599547
C	1.2598772642	19.6625552628	2.3553314699	C	1.2589022904	19.6689732204	2.3753809998
C	0.0267972289	17.5359355543	2.3455706384	C	0.0282292233	17.5413365377	2.3484269356
C	1.2418774586	18.2515755282	2.3525389632	C	1.2428161494	18.2581160479	2.3678385124
C	2.4948816029	20.3672677120	2.3560133144	C	2.4898637696	20.3812497791	2.3741855239
C	0.0278455136	16.1126102820	2.3411930739	C	0.0309029735	16.1188898836	2.3433131526

H	2.1814129275	17.7025496321	2.3536997910	H	2.1825839997	17.7089309421	2.3697824850
C	3.5642926319	20.9746152065	2.3527734071	C	3.5506447927	21.0034364522	2.3616558296
C	0.0228127674	14.8823311193	2.3383359107	C	0.0257700027	14.8890469088	2.3451667311
C	-8.1859901423	20.7915093671	2.3334991900	C	-8.1799606552	20.7732337661	2.3365644970
O	-8.1699883113	20.1266376307	1.3170253862	O	-8.1496353610	20.1105986969	1.3189176914
O	-8.1906251689	20.2704847091	3.5863501846	O	-8.1938875851	20.2484401184	3.5876333695
H	-8.1712833067	19.2948358190	3.4889483203	H	-8.1609225463	19.2733463711	3.4864365576
C	-2.4956459752	17.5158997367	2.3916017216	C	-2.4986187831	17.5208278976	2.3612498939
O	-3.0643126628	17.2081430734	3.4200987066	O	-3.1193154437	17.2678741655	3.3744902301
O	-2.9606196530	17.2346706125	1.1486547416	O	-2.9051677361	17.1792017947	1.1126355947
H	-3.8099680957	16.7580329925	1.2638196288	H	-3.7654998359	16.7181146620	1.2099541608
C	15.2610622504	10.1548264264	2.3327899436	C	15.2342951448	10.1320443783	2.3433459072
H	14.3152236310	10.6929086479	2.3269014784	H	14.2831108436	10.6607535468	2.3406799950
C	15.2493107676	8.7447696293	2.3466901433	C	15.2357756511	8.7218739304	2.3549653982
C	14.0165824393	8.0376506893	2.3510922566	C	14.0086060064	8.0030866922	2.3590167672
C	12.9524529611	7.4222533224	2.3519033775	C	12.9472505910	7.3825282181	2.3631365367
C	16.4740426529	10.8751891171	2.3322448550	C	16.4406960295	10.8635600206	2.3409185494
C	16.4712991337	12.2981053947	2.3351301635	C	16.4237942614	12.2863106908	2.3423163984
C	16.4716654315	13.5281954972	2.3417343428	C	16.4118469408	13.5163111274	2.3444528187
C	17.6903367140	10.1604830293	2.3341016647	C	17.6650556874	10.1619798531	2.3387686127
C	16.4808455685	8.0465144147	2.3591249134	C	16.4753898577	8.0364980715	2.3635542683
C	23.4760086776	5.4234815276	2.3480427734	C	23.4784963057	5.4438134412	2.3606534261
C	17.7094788246	8.7506586772	2.3470352525	C	17.6983317427	8.7521944951	2.3492862991
H	18.6340719875	10.7025083287	2.3292955733	H	18.6021474839	10.7156964714	2.3314993775
C	22.2494576277	6.1426153905	2.3451342758	C	22.2539610255	6.1672334483	2.3547108756
C	18.9455393167	8.0482786479	2.3501127671	C	18.9416753514	8.0606443804	2.3489273714
C	21.1847038134	6.7574585827	2.3446447759	C	21.1890565774	6.7821978941	2.3496411250
C	20.0107471464	7.4342597180	2.3470556169	C	20.0121470323	7.4551435513	2.3486080748
C	23.4802001827	4.0072077836	2.3424792801	C	23.4765316128	4.0269917212	2.3416859380
C	24.7059976806	6.1118354110	2.3546227871	C	24.7113308205	6.1275553878	2.3769798121
H	24.7047286820	7.2001327533	2.3576775185	H	24.7140396498	7.2160446805	2.3887770057
C	25.9315853488	5.4135737846	2.3554271051	C	25.9350792229	5.4255358388	2.3776799950
C	24.6999110518	3.2874350029	2.3466890251	C	24.6939288047	3.3026935587	2.3505041814
C	25.9148865526	4.0029800816	2.3534730676	C	25.9116387320	4.0147806375	2.3705635720
C	27.1642836996	6.1219189598	2.3560690220	C	27.1706415322	6.1308421763	2.3812567114
C	24.6996554266	1.8650333900	2.3420691751	C	24.6910513374	1.8797072735	2.3461544408

H	26.8546919717	3.4540873773	2.3553779335	H	26.8487344870	3.4616216801	2.3799403506
C	28.2291311259	6.7363917506	2.3544216484	C	28.2355688927	6.7462887817	2.3753581071
C	24.6883760116	0.6355390478	2.3353140606	C	24.6836502437	0.6496211201	2.3448154993
C	16.4889857456	6.5459750054	2.3336615176	C	16.4972166478	6.5362153819	2.3357618464
O	16.5012771387	5.8819903610	1.3165355295	O	16.5380787088	5.8741998185	1.3181127077
O	16.4852435426	6.0241933804	3.5860329498	O	16.4689477336	6.0117889382	3.5865468508
H	16.5017515613	5.0485281936	3.4880868462	H	16.4944045747	5.0362884071	3.4862429198
C	22.1766211268	3.2657635270	2.3909665282	C	22.1669565596	3.2941784876	2.3644977605
O	21.6053275841	2.9630193878	3.4195939104	O	21.5334143749	3.0617994751	3.3747891130
O	21.7132066374	2.9804682423	1.1484921516	O	21.7741513760	2.9296221460	1.1182561325
H	20.8612347187	2.5087953866	1.2646811098	H	20.9154382766	2.4658580928	1.2167511697
C	7.0320773709	24.3906080877	2.3216574714	C	7.0280140335	24.4025964679	2.3234043334
H	6.0819035090	24.9212648402	2.3131491216	H	6.0767288368	24.9317118238	2.3151464867
C	7.0320468980	22.9799664781	2.3424114120	C	7.0278352481	22.9923060692	2.3304909809
C	5.8041752514	22.2641747804	2.3487770904	C	5.7939974292	22.2864586168	2.3356473600
C	4.7397488797	21.6488108352	2.3497493867	C	4.7229735700	21.6833245970	2.3495094268
C	8.2382895638	25.1216669633	2.3190349660	C	8.2339223258	25.1346897868	2.3352552308
C	8.2268873723	26.5442806069	2.3196875704	C	8.2221172103	26.5573047280	2.3358013321
C	8.2294780962	27.7740058901	2.3279369468	C	8.2261990896	27.7876661998	2.3410444108
C	9.4610807239	24.4188230696	2.3239383854	C	9.4571470470	24.4315195913	2.3511492965
C	8.2695644129	22.2931758183	2.3645202977	C	8.2670701282	22.3013043555	2.3692775553
C	15.2530677129	19.6778922022	2.3578479286	C	15.2466668872	19.6805285778	2.3566096579
C	9.4914207621	23.0105035621	2.3481404991	C	9.4904051781	23.0226904948	2.3739005097
H	10.3998922297	24.9696378651	2.3148899538	H	10.3946414078	24.9839711589	2.3497758583
C	14.0297054933	20.4016360816	2.3539287141	C	14.0348740278	20.4234078779	2.3537300494
C	10.7324803636	22.3179789435	2.3572988444	C	10.7416518753	22.3462010423	2.3676627547
C	12.9688548043	21.0230122153	2.3550286680	C	12.9843336619	21.0624937613	2.3505097275
C	11.7977324871	21.7044087880	2.3566186197	C	11.8154316073	21.7477157734	2.3518931354
C	15.2536545402	18.2609362314	2.3534851778	C	15.2268443791	18.2640600332	2.3367637348
C	16.4844616635	20.3631229729	2.3606816982	C	16.4888552396	20.3458584402	2.3678096412
H	16.4863480462	21.4514455538	2.3636100450	H	16.5075700331	21.4337671364	2.3752068940
C	17.7081773307	19.6620064353	2.3603272800	C	17.7028988859	19.6276759197	2.3640430098
C	16.4715097150	17.5375980785	2.3516617511	C	16.4341920709	17.5240151337	2.3423119196
C	17.6880914677	18.2512767014	2.3575093245	C	17.6626139510	18.2177727931	2.3581233939
C	18.9407825032	20.3700264902	2.3563139040	C	18.9438784216	20.3215255880	2.3613409612
C	16.4727345161	16.1146427039	2.3486737967	C	16.4159353069	16.1020119951	2.3383139130

H	18.6263421383	17.7000930472	2.3599773372	H	18.5927953316	17.6521277593	2.3595191537
C	20.0030392262	20.9890077709	2.3491078217	C	20.0078389447	20.9380764736	2.3556545666
C	16.4727629701	14.8846678295	2.3472593897	C	16.4090836322	14.8722615363	2.3429803691
C	8.3121721892	20.7917664552	2.3727291226	C	8.2802708858	20.8030908830	2.3695406042
O	8.3204350570	20.1052288381	1.3696142043	O	7.8128359588	20.1124843466	1.4840825815
O	8.3673083739	20.3093154056	3.6356079441	O	8.8851303680	20.3160229644	3.4808947725
H	8.4741044829	19.3332250164	3.5811489113	H	8.9475650081	19.3370507385	3.3912989011
C	13.9442113280	17.5307682238	2.4087506295	C	13.9075735668	17.5516306061	2.3583869648
O	13.3378649708	17.2967336332	3.4357639326	O	13.2661588419	17.3326232417	3.3680052845
O	13.5141212104	17.1743274693	1.1730433283	O	13.5105924705	17.1917223547	1.1132600373
H	12.6563463382	16.7138333900	1.2926192715	H	12.6427928349	16.7444347651	1.2079668168
N	9.5036333568	17.3708456692	3.7826449241	N	10.1773979989	17.5578936803	3.9174421076
N	10.1033332989	16.4444471633	3.6686195386	O	10.6291968063	17.3483251423	4.9662297622
COOH-HsGDY + N₂O adsorbed system				COOH-HsGDY + NO₂ adsorbed system			
C	-1.1793737046	10.1523044582	2.3413832575	C	-1.1848892941	10.1452714421	2.3469060947
H	-2.1285325622	10.6844691833	2.3346526050	H	-2.1346224279	10.6763273597	2.3462249788
C	-1.1822519911	8.7423486686	2.3544082727	C	-1.1886206959	8.7347264412	2.3555152762
C	-2.4115706744	8.0286199039	2.3576654430	C	-2.4179761392	8.0210159497	2.3570894198
C	-3.4755101943	7.4123640853	2.3558243421	C	-3.4815520198	7.4035960878	2.3558695956
C	0.0277679015	10.8812946420	2.3377287158	C	0.0232209539	10.8739252055	2.3433330953
C	0.0171796883	12.3034942154	2.3346113506	C	0.0149835299	12.2970394493	2.3423348155
C	0.0159641080	13.5334041741	2.3381690379	C	0.0197618550	13.5277382133	2.3436813553
C	1.2498890549	10.1765407213	2.3371418389	C	1.2440569488	10.1657683965	2.3410924270
C	0.0550348497	8.0539177818	2.3576006293	C	0.0472034551	8.0430853058	2.3607137601
C	7.0280033293	5.4129463056	2.3471885624	C	7.0278479982	5.4116915123	2.3449133976
C	1.2785987761	8.7675163900	2.3436423326	C	1.2714612545	8.7559589965	2.3485476332
H	2.1888213266	10.7270837146	2.3345692320	H	2.1842341191	10.7140712621	2.3383145328
C	5.8082476613	6.1430920881	2.3438849336	C	5.8052169071	6.1372552379	2.3426797805
C	2.5182269441	8.0718462650	2.3466784689	C	2.5102006003	8.0586117366	2.3499545300
C	4.7493196850	6.7678261948	2.3455152498	C	4.7442912292	6.7590262663	2.3449879589
C	3.5811145083	7.4542973819	2.3474841101	C	3.5738873159	7.4415866283	2.3490766929
C	7.0197235215	3.9965590182	2.3350861583	C	7.0252272445	3.9948741320	2.3319025335
C	8.2643426740	6.0901134894	2.3586315277	C	8.2618583837	6.0936141250	2.3551926420
H	8.2737296044	7.1785530305	2.3654526781	H	8.2676783645	7.1819996451	2.3603564899
C	9.4843877170	5.3817757946	2.3601085549	C	9.4844665184	5.3893396045	2.3523770950
C	8.2332308771	3.2666156725	2.3454561180	C	8.2416676629	3.2691346870	2.3420323568

C	9.4550793673	3.9713116841	2.3588743705	C	9.4605447331	3.9786171810	2.3509122896
C	10.7218228692	6.0836157795	2.3601084219	C	10.7197837573	6.0927319850	2.3497451010
C	8.2235868709	1.8443933151	2.3395146336	C	8.2363932142	1.8469254649	2.3414730171
H	10.3893173476	3.4126550593	2.3605706030	H	10.3972784985	3.4244121251	2.3497372512
C	11.7855424934	6.7015098231	2.3554279596	C	11.7850604150	6.7076429045	2.3474613769
C	8.2176554375	0.6145822943	2.3440387266	C	8.2291119712	0.6167243176	2.3451880941
C	0.0776928621	6.5544132504	2.3267967681	C	0.0652335096	6.5423585509	2.3314304494
O	0.1864698100	5.8956138597	1.3118977584	O	0.1188300603	5.8810531229	1.3138521536
O	-0.0316852647	6.0256744094	3.5713996985	O	0.0190867109	6.0176240493	3.5813489868
H	-0.0014375744	5.0508237382	3.4681292734	H	0.0429370976	5.0420833946	3.4817860846
C	5.7091108899	3.2644950735	2.3566554070	C	5.7182773479	3.2574837398	2.3548834897
O	5.1097985442	2.9686395738	3.3710294266	O	5.1205848985	2.9631520278	3.3707063849
O	5.2757370892	2.9762527547	1.1038015583	O	5.2872863265	2.9640568888	1.1026867832
H	4.4192763083	2.5073095368	1.2000568569	H	4.4330570466	2.4913128749	1.1983890053
C	-9.4342722224	24.3731236906	2.4044855385	C	-9.4304801676	24.3783541259	2.3276838339
H	-10.3819031549	24.9079004783	2.4234010252	H	-10.3773037405	24.9152917291	2.3169702708
C	-9.4410771511	22.9623062056	2.4199050732	C	-9.4394173494	22.9675933423	2.3352173210
C	-10.6735036716	22.2497521122	2.4386186588	C	-10.6687221265	22.2544215628	2.3233274472
C	-11.7363364195	21.6301035745	2.4358489188	C	-11.7251040918	21.6247749455	2.3094213804
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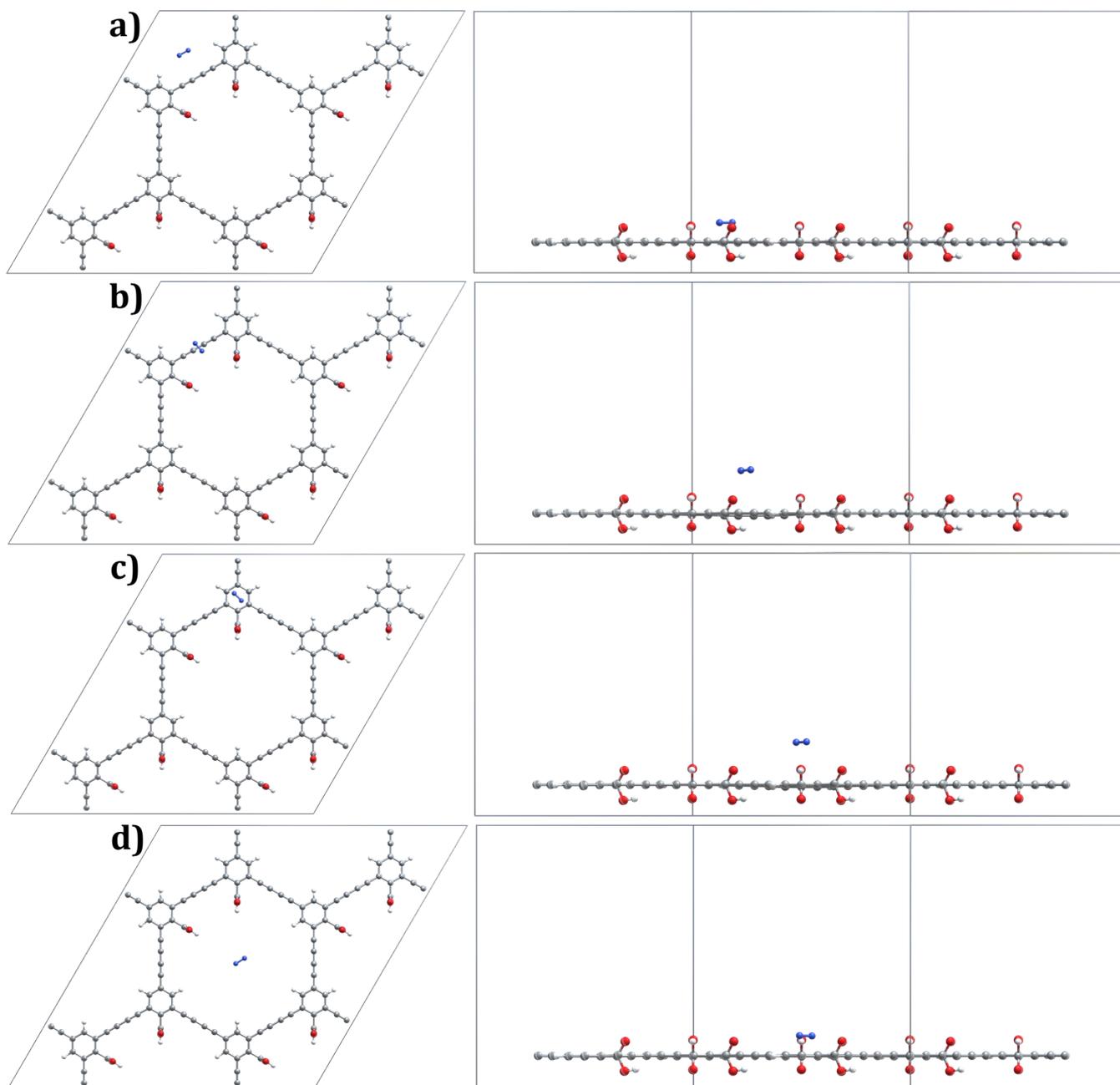
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H	-8.2408128623	19.2559044074	3.4796232826	H	-8.2455121253	19.2736132360	3.4760682966
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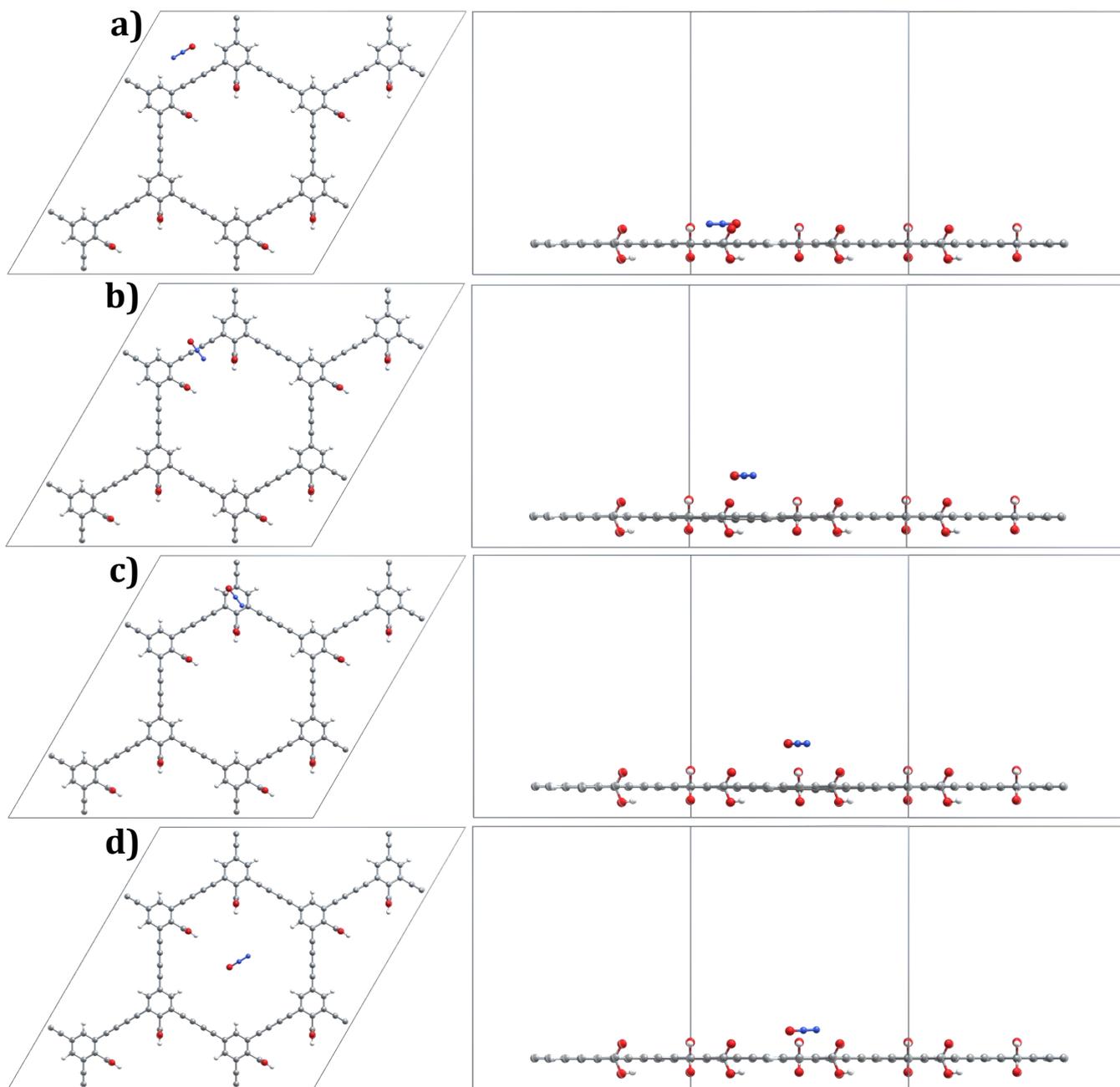
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O	8.2080131608	20.3624214819	3.7821142616	O	9.0827250626	20.2856005447	3.4371046296
H	8.3781406005	19.3937568922	3.7612602971	H	9.1120888432	19.2920288118	3.3768426610
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O	10.7422390805	16.0188862572	2.3236665595	O	10.5398395880	16.5275244654	2.2544684810

SIT4. The adsorption Energies (E_{ads}) of nitrogen and its oxides at different sites over COOH-HsGDY slab

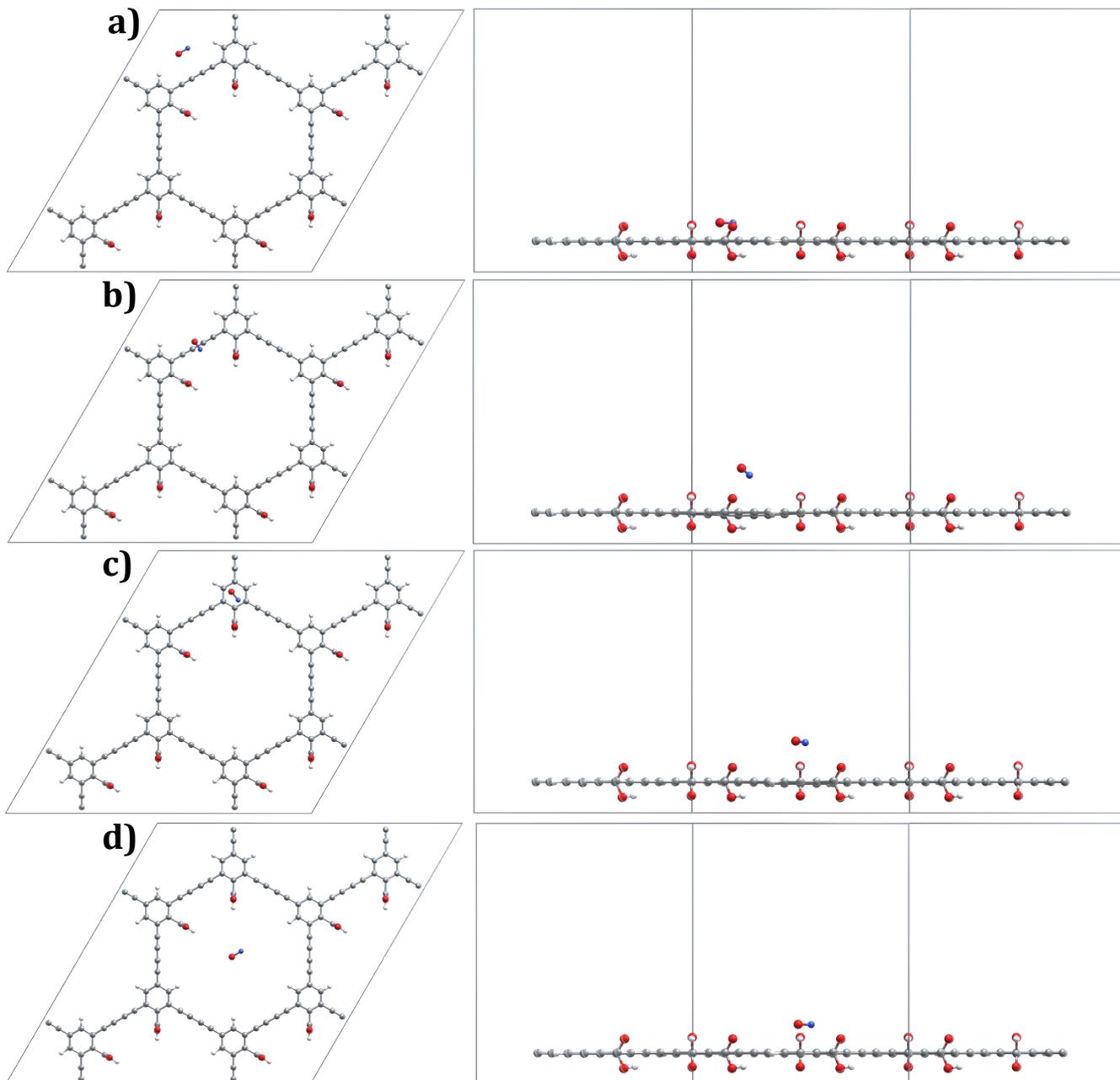
E_{ads} (eV)	Adsorption Sites	N_2	N_2O	NO	NO_2
	Site 1	-0.084	-0.118	-0.084	-0.163
	Site 2	-0.137	-0.291	-0.159	-0.493
	Site 3	-0.060	-0.098	-0.072	-0.132
	Site 4	-0.084	-0.092	-0.098	-0.159
	Site 5	-0.002	-0.001	-0.005	-0.083



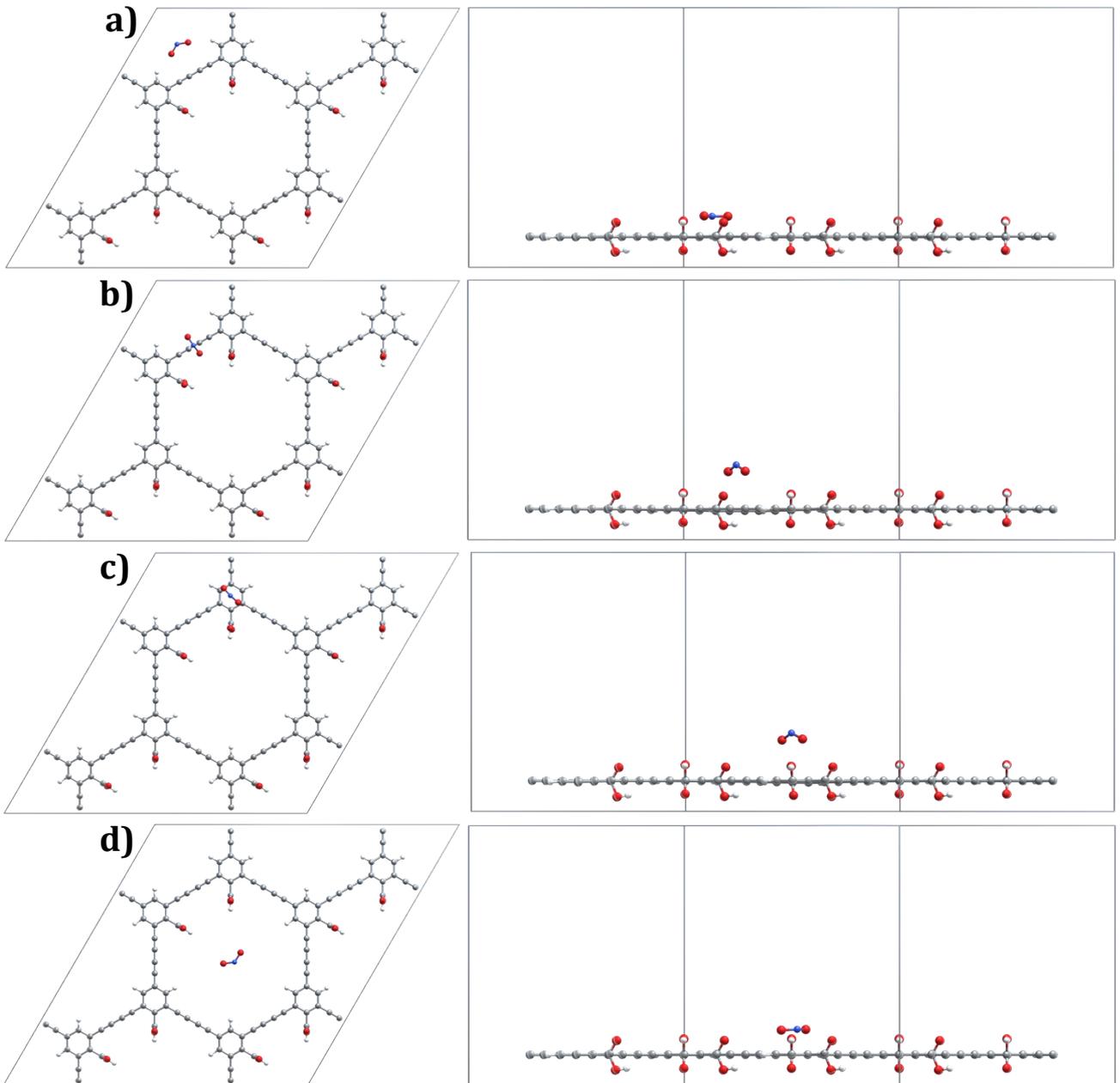
SIF2. Top view and side view of the N_2 adsorbed a) S1, b) S3, c) S4, and d) S5 onto COOH-HsGDY.



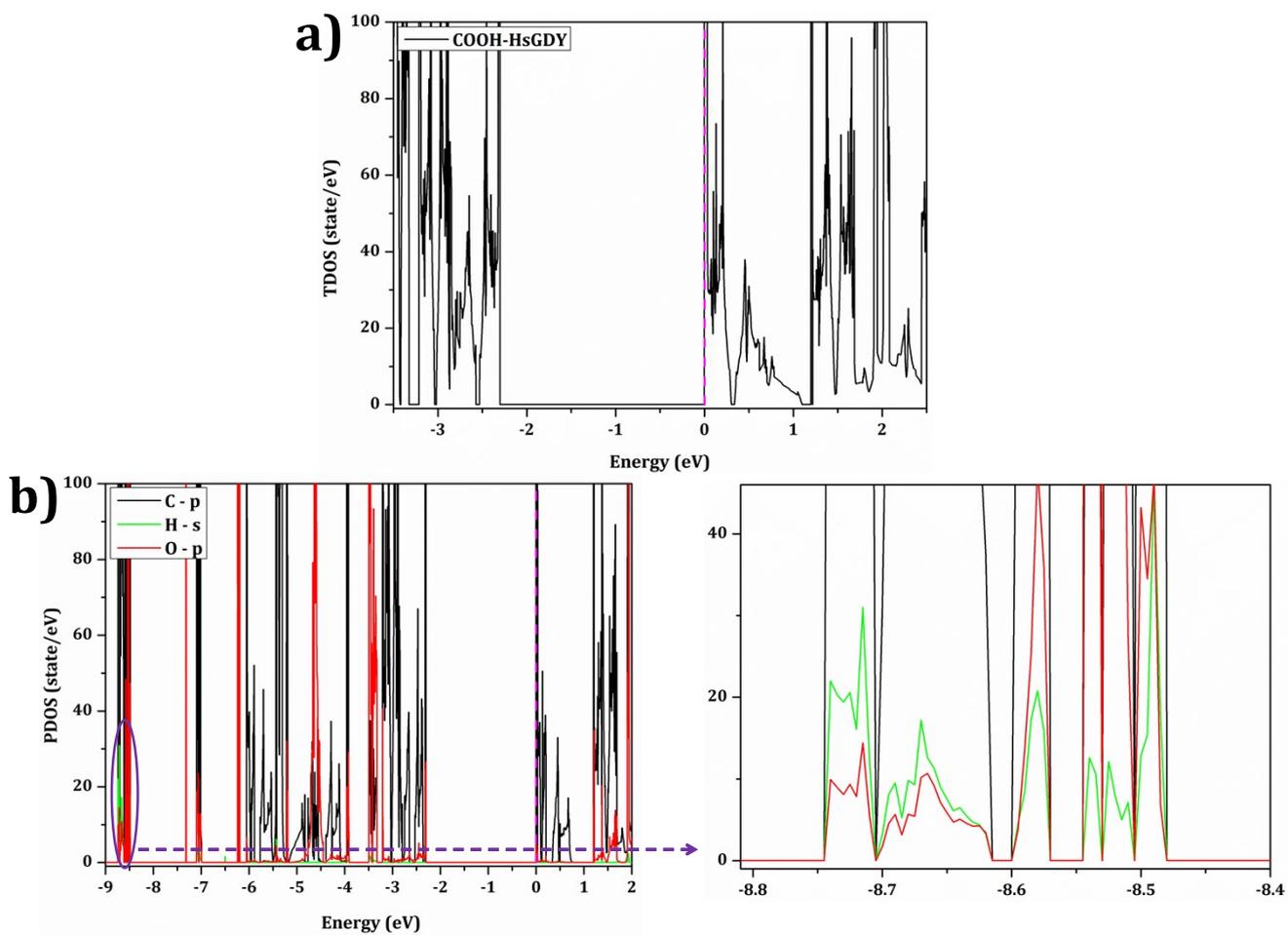
SIF3. Top view and side view of the N₂O adsorbed a) S1, b) S3, c) S4, and d) S5 onto COOH-HsGDY.



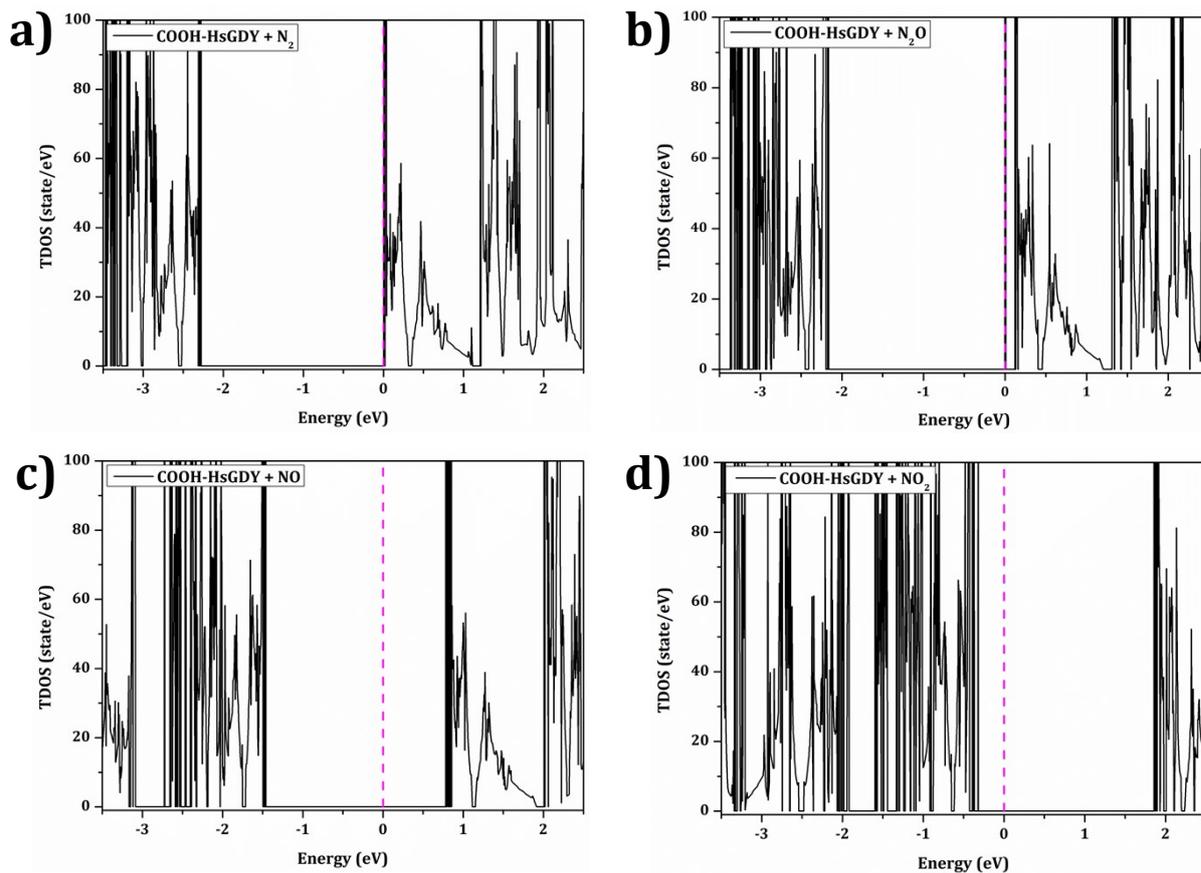
SIF4. Top view and side view of the NO adsorbed a) S1, b) S3, c) S4, and d) S5 onto COOH-HsGDY.



SIF5. Top view and side view of the NO_2 adsorbed a) S1, b) S3, c) S4, and d) S5 onto COOH-HsGDY.



SIF6. a) and b) are the TDOS and PDOS of COOH-HsGDY slab. The pink dashed line denotes the Fermi level, which has been set to 0 eV.



SIF7. TDOS of (a) N₂, (b) N₂O, (c) NO, and (d) NO₂ gas molecules adsorbed onto COOH-HsGDY. The pink dashed line denotes the Fermi level, which has been set to 0 eV.