

Robust and facile detection of formaldehyde through transition metals doped olympicene sensors: A step forward DFT investigation

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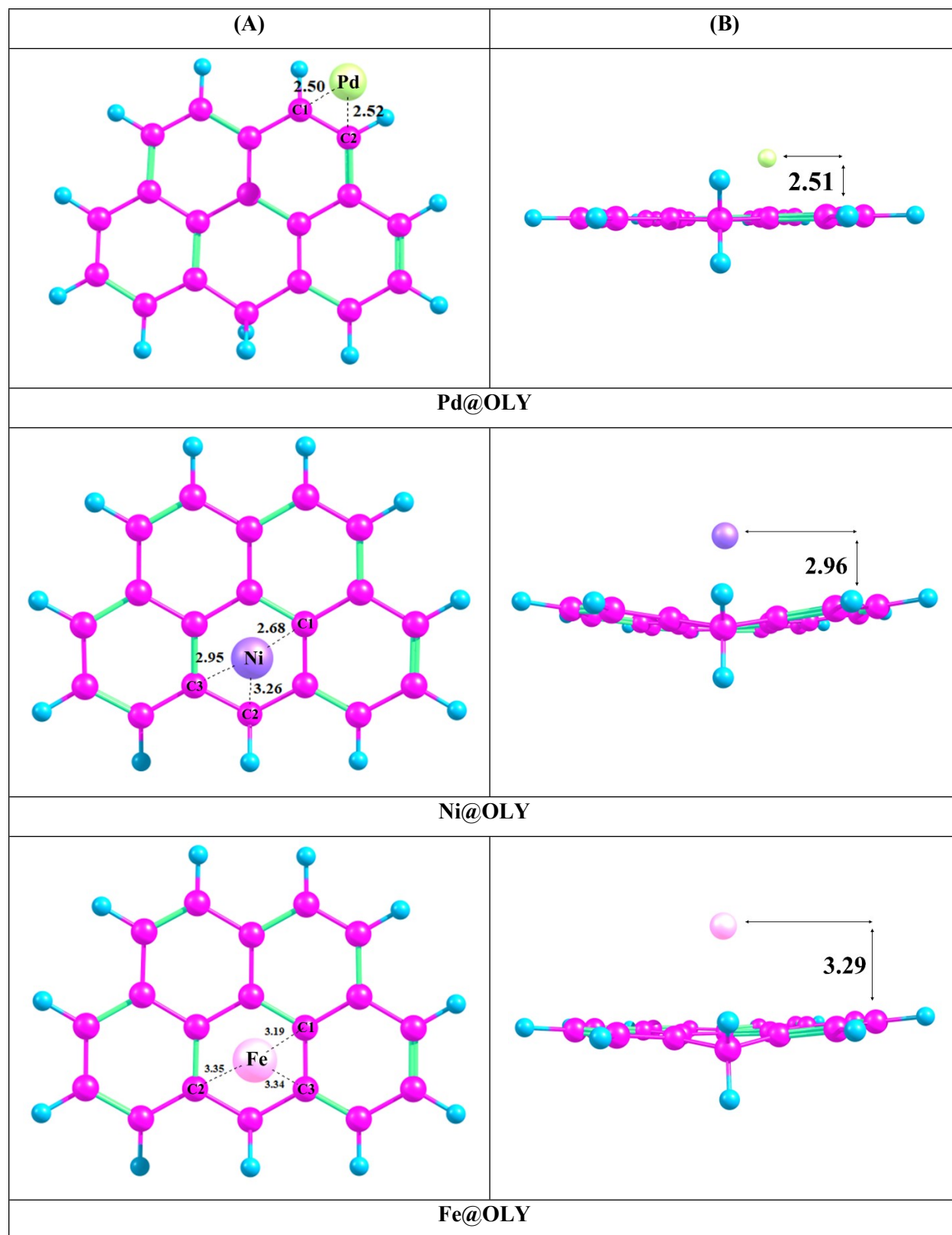


Figure S1: (A) Optimized geometries and bond distances of TM@olypicene complexes (B) Average distance between TM and Olypicene

Table S1: Interaction energies and shortest bond distances of TM@olympicene

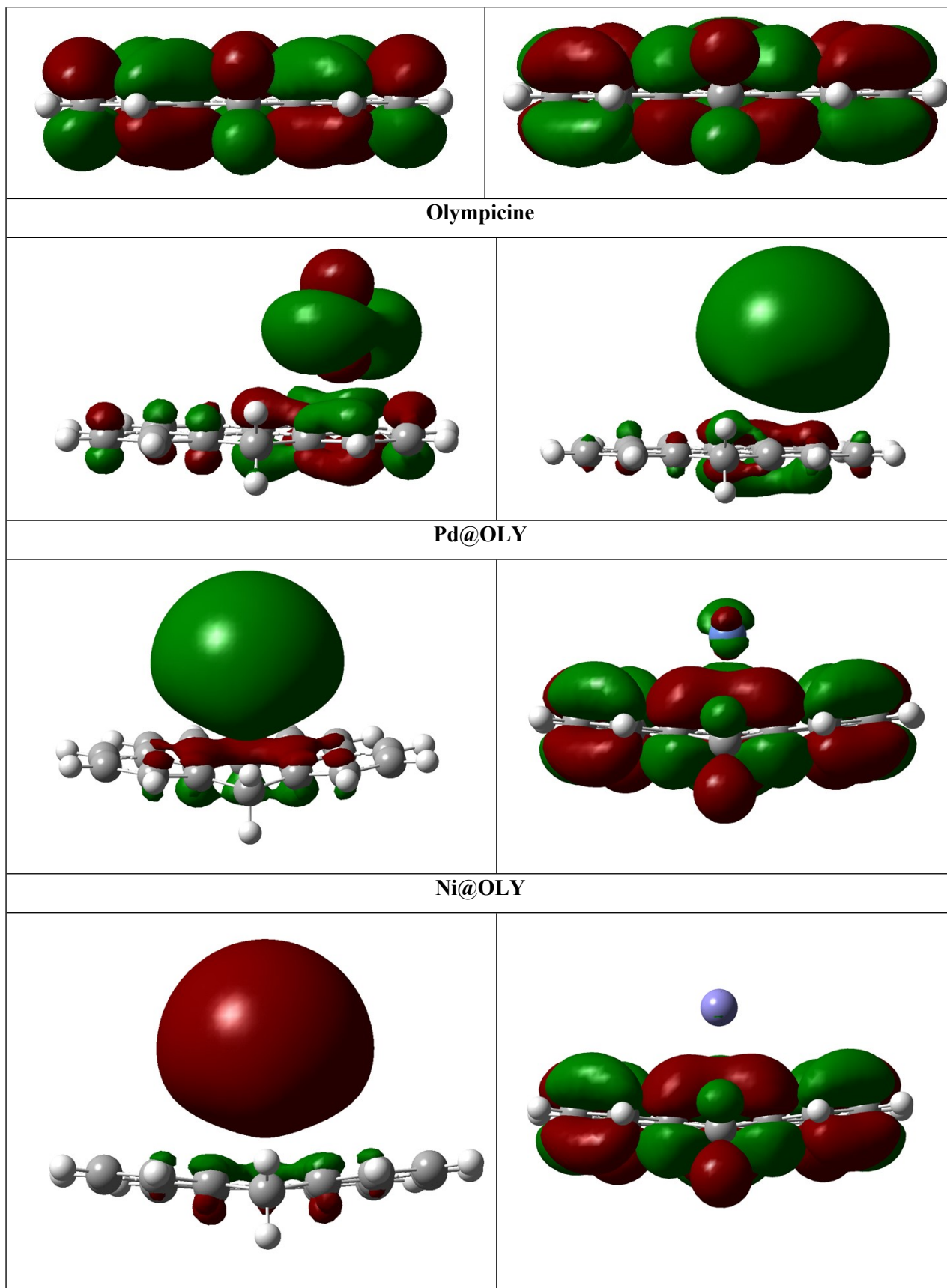
Complexes	Interaction energy (E_{in}) (kcal/mol)	BSSE corrected energy (kcal/mol)	BSSE correction energy (kcal/mol)	closest interacting atoms	Q_{NBO} (TM)	D_{int}	Average distance (TM@OLY)
Pd@OLY	-27.19	-25.68	1.52	Pd-C1	0.103	2.50	2.51
Ni@OLY	-11.62	-11.15	0.47	Ni-C1	0.050	2.68	2.96
Fe@OLY	-30.08	-31.89	-0.43	Fe-C1	- 0.004	3.19	3.29
Ti@OLY	-137.01	-135.28	1.73	--	--	--	--

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Table S2: All BCPs values of TM@OLY and OLY(TM)/HCHO from QTAIM analysis

HCHO/(TM)OLY	OLY-analyte	BCPs	ρ	$\nabla^2 \rho$	G(r)	V(r)	H(r)	-V/G
Pd@OLY	C-Pd	49	0.044	0.130	0.038	-0.043	-0.0054	1.13
Ni@OLY	C-Ni	49	0.025	0.067	0.019	-0.021	-0.0021	1.10
Fe@OLY	C-Fe	35	0.011	0.022	0.005	-0.006	-0.0002	1.20
HCHO/(Ni)OLY	Ni4-O2	56	0.115	0.666	0.197	-0.228	-0.0309	1.15
	C3-H1	66	0.004	0.014	0.003	-0.002	0.0006	0.66
HCHO/(Fe)OLY	Fe2-C4	52	0.039	0.059	0.020	-0.025	-0.0054	1.25
	C3-O1	76	0.009	0.041	0.008	-0.006	0.0020	0.75
HCHO/(Pd)OLY	Pd4-O3	40	0.040	0.108	0.032	-0.037	-0.0048	1.15
	C2-H1	51	0.006	0.018	0.003	-0.003	0.0007	1.00

HOMO	LUMO
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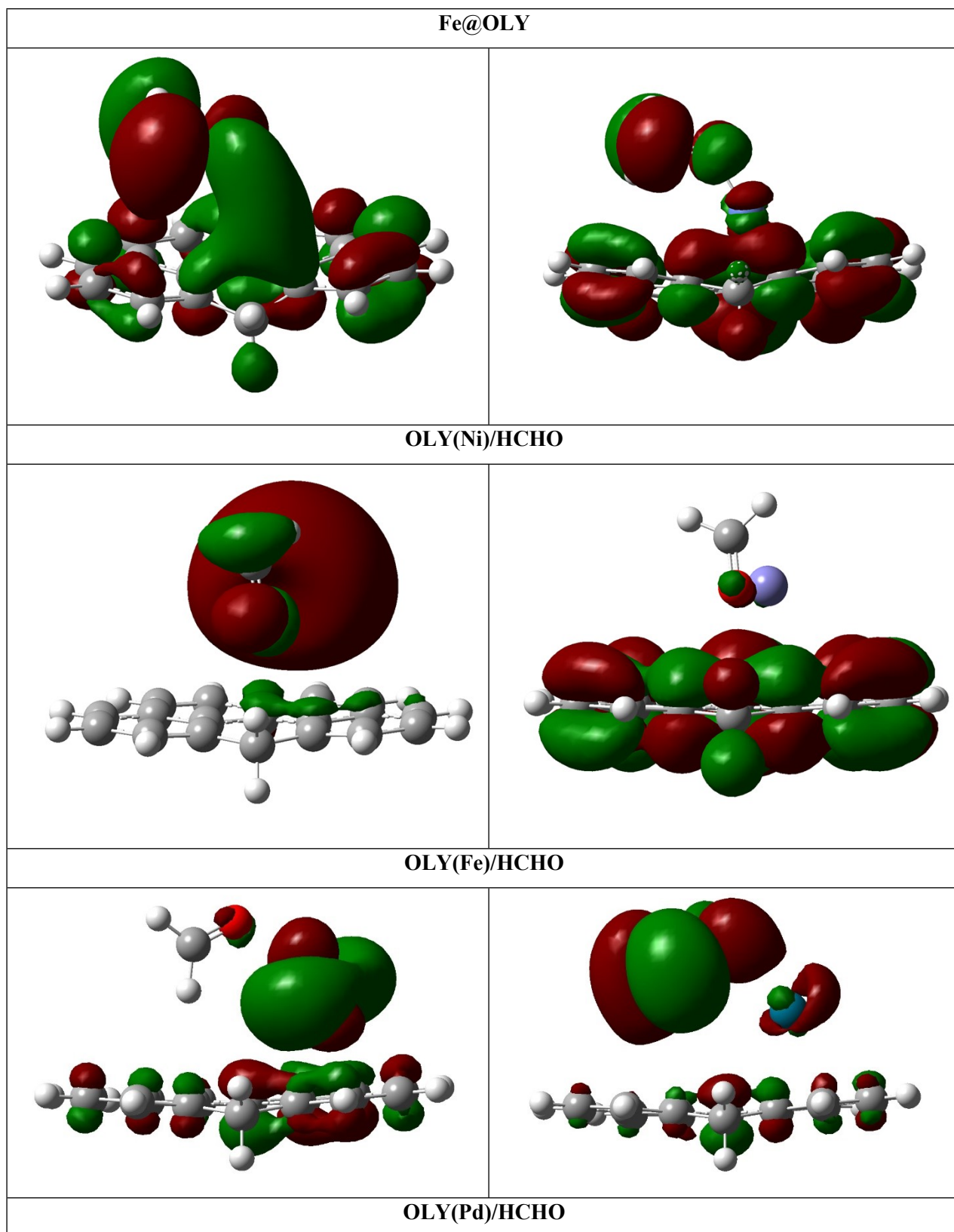
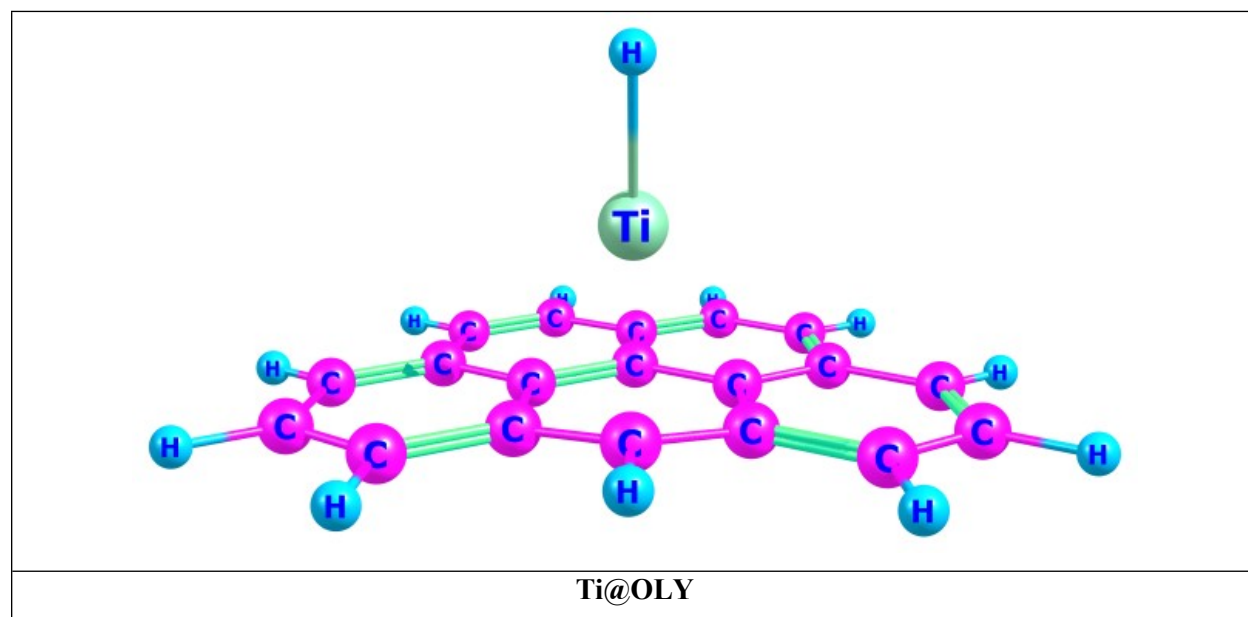


Figure S2: HOMO–LUMO iso surfaces of olympicene, TM@OLY and OLY(TM)/HCHO complexes.

Table S3: Selectivity of TM doped olympicene over water, nitrogen and oxygen

Complexes	E _{HOMO} (eV)	E _{LUMO} (eV)	E _{H-L} gap (eV)	E _{int}
OLY	-5.51	-1.49	4.01	-
Pd@OLY	-4.81	-1.81	2.99	-25.98
Ni@OLY	-3.88	-1.74	2.14	-12.61
Fe@OLY	-4.62	-1.70	2.90	-7.26
OLY(Ni)/N ₂	-3.90	-1.76	2.14	-0.16
OLY(Ni)/O ₂	-4.66	-2.15	2.51	-2.67
OLY(Ni)/H ₂ O	3.46	6.54	3.08	-0.51
OLY(Fe)/N ₂	3.46	6.54	3.08	-2.40
OLY(Fe)/O ₂	-4.90	-2.23	2.67	-88.79
OLY(Fe)/H ₂ O	-3.95	-1.69	2.26	-12.47
OLY(Pd)/N ₂	-5.31	-1.80	3.50	-1.12
OLY(Pd)/O ₂	-5.08	-2.68	2.40	-2.34
OLY(Pd)/H ₂ O	-4.97	-1.84	3.13	-0.38
Ti@OLY	-4.66	-2.28	2.38	-39.69
OLY(Ti)FMH	-4.58	-2.17	2.40	-36.92

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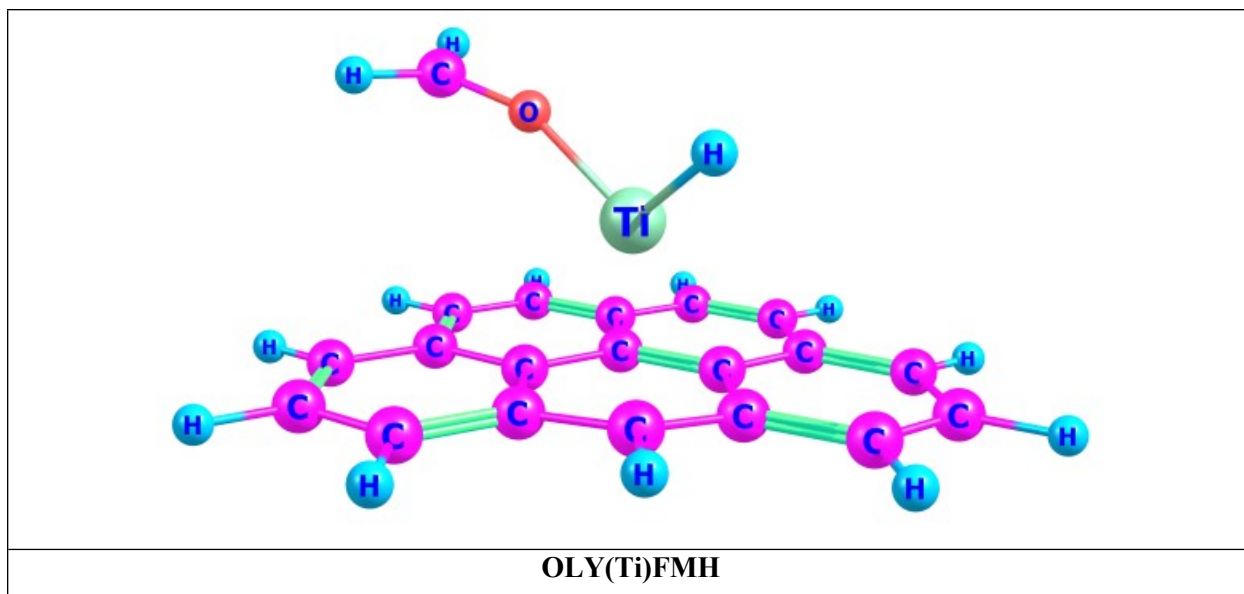
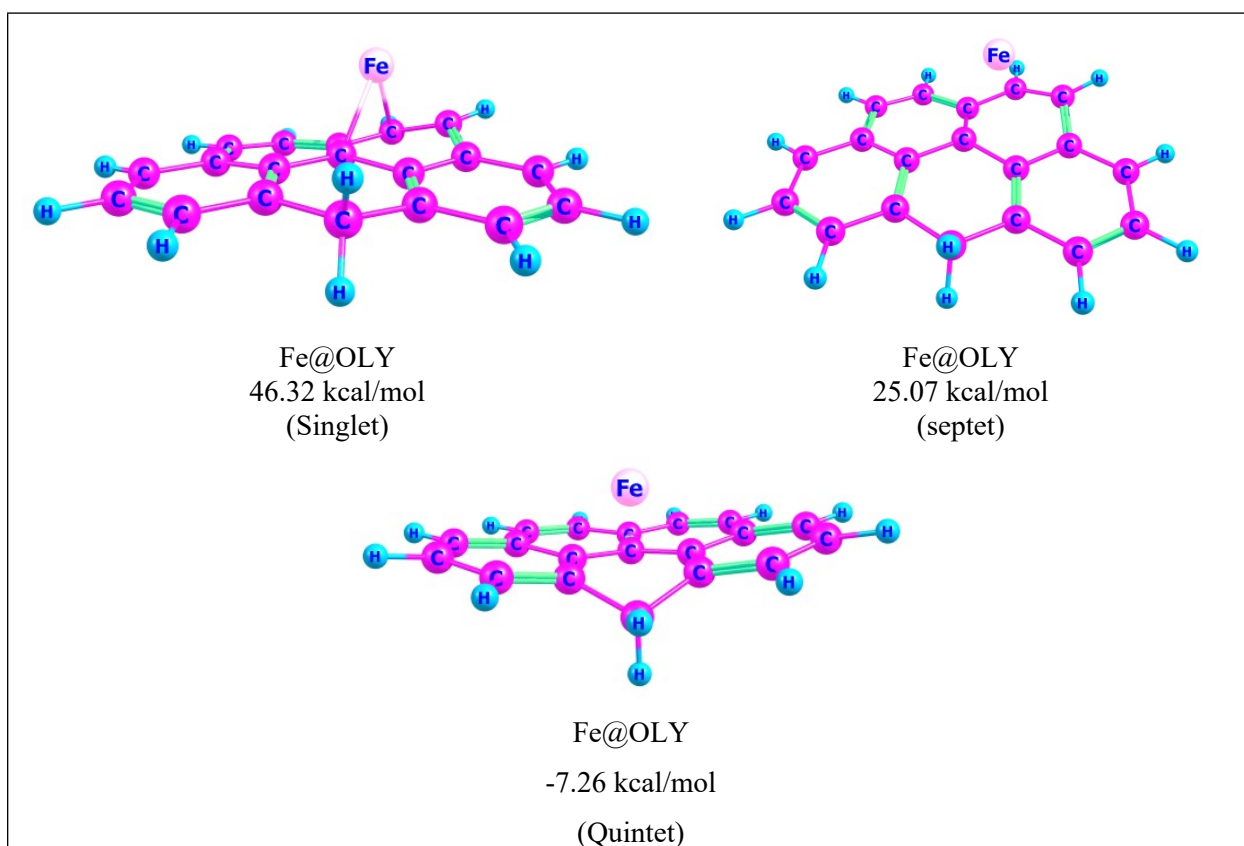
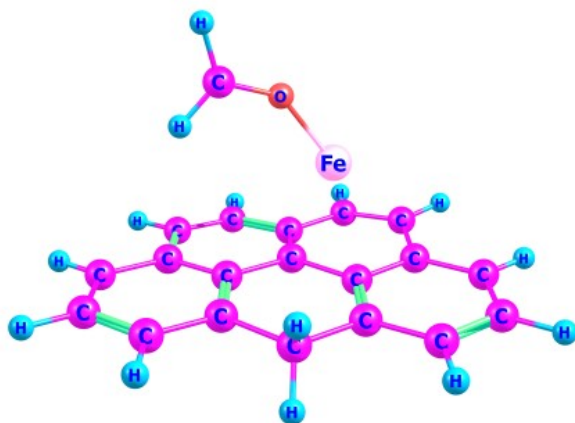
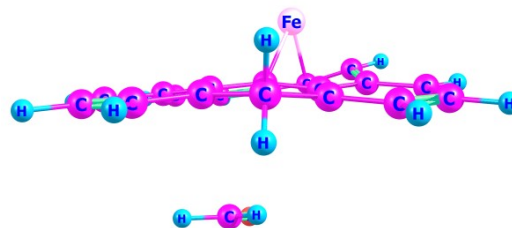


Figure S3: Optimized geometry of Ti@OLY and OLY(Ti)FMH

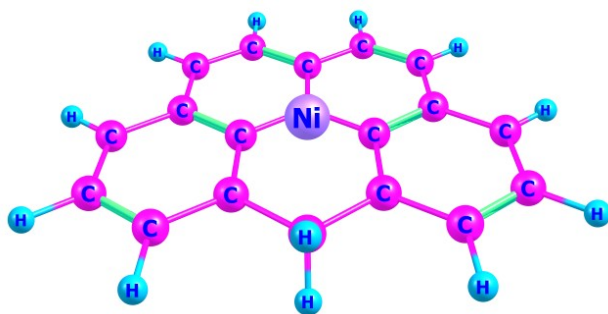




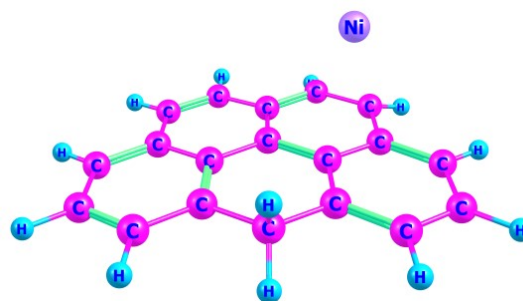
OLY(Fe)FMH
-10.70 kcal/mol



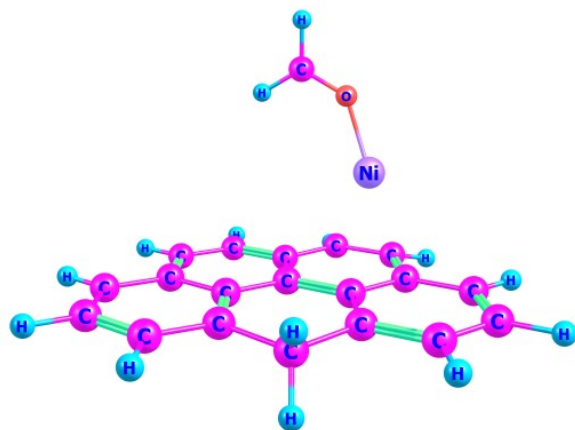
OLY(Fe)FMH
27.97 kcal/mol



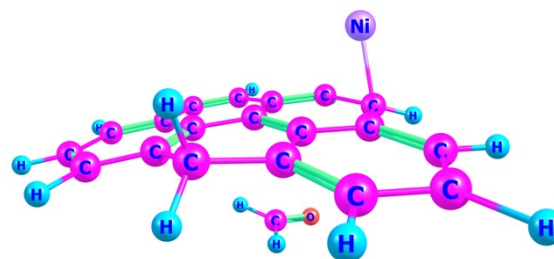
Ni@OLY
-10.21 kcal/mol
(Quintet)



Ni@OLY
-12.61 kcal/mol
(Triplet)



OLY(Ni)FMH
-12.50 kcal/mol



OLY(Ni)FMH
-5.61 kcal/mol

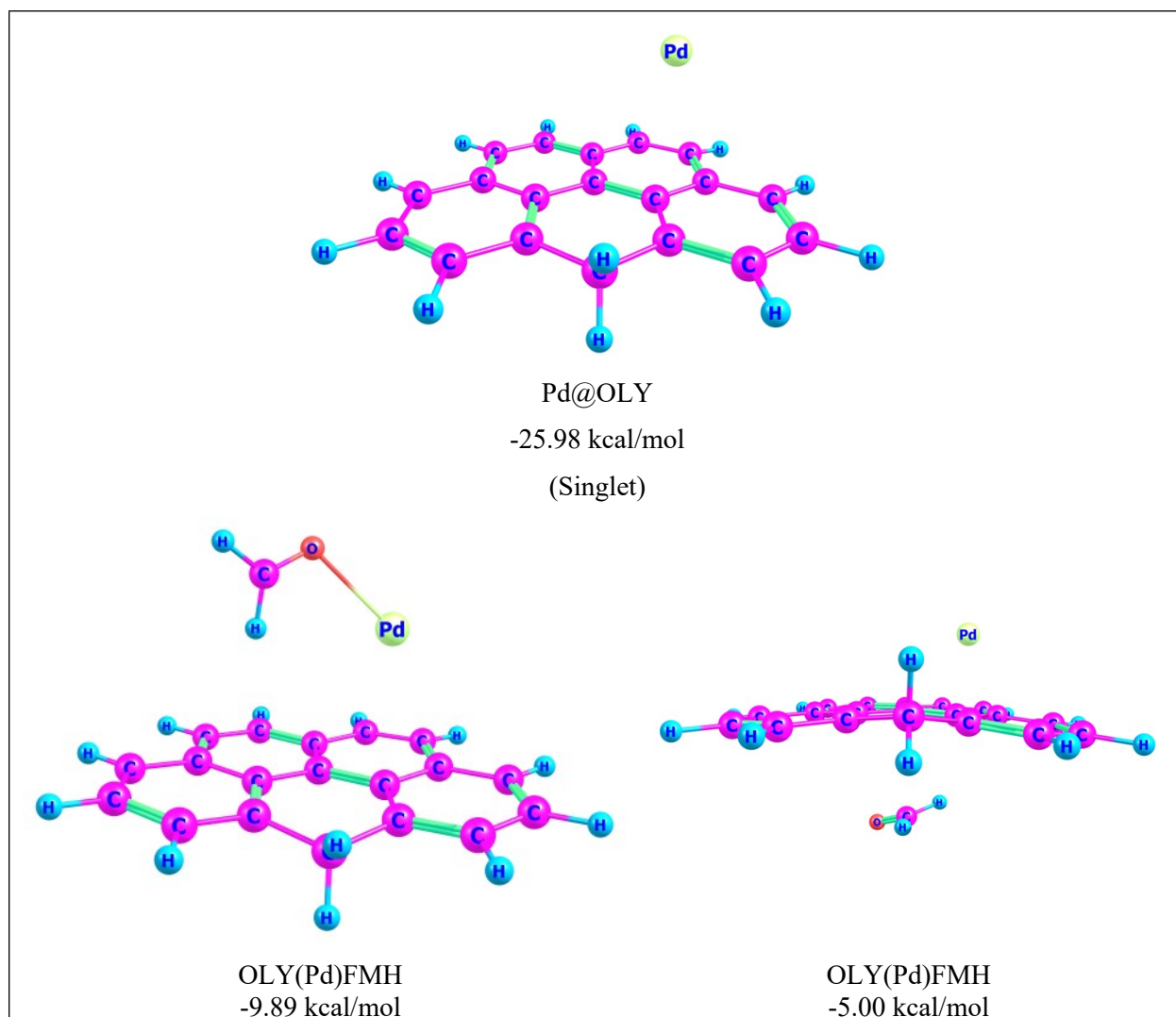
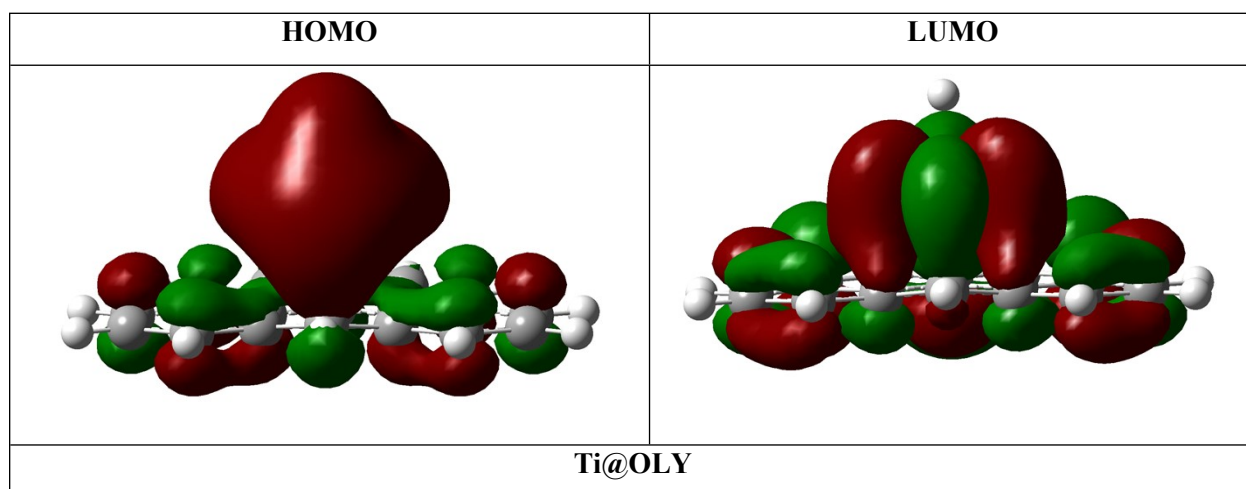
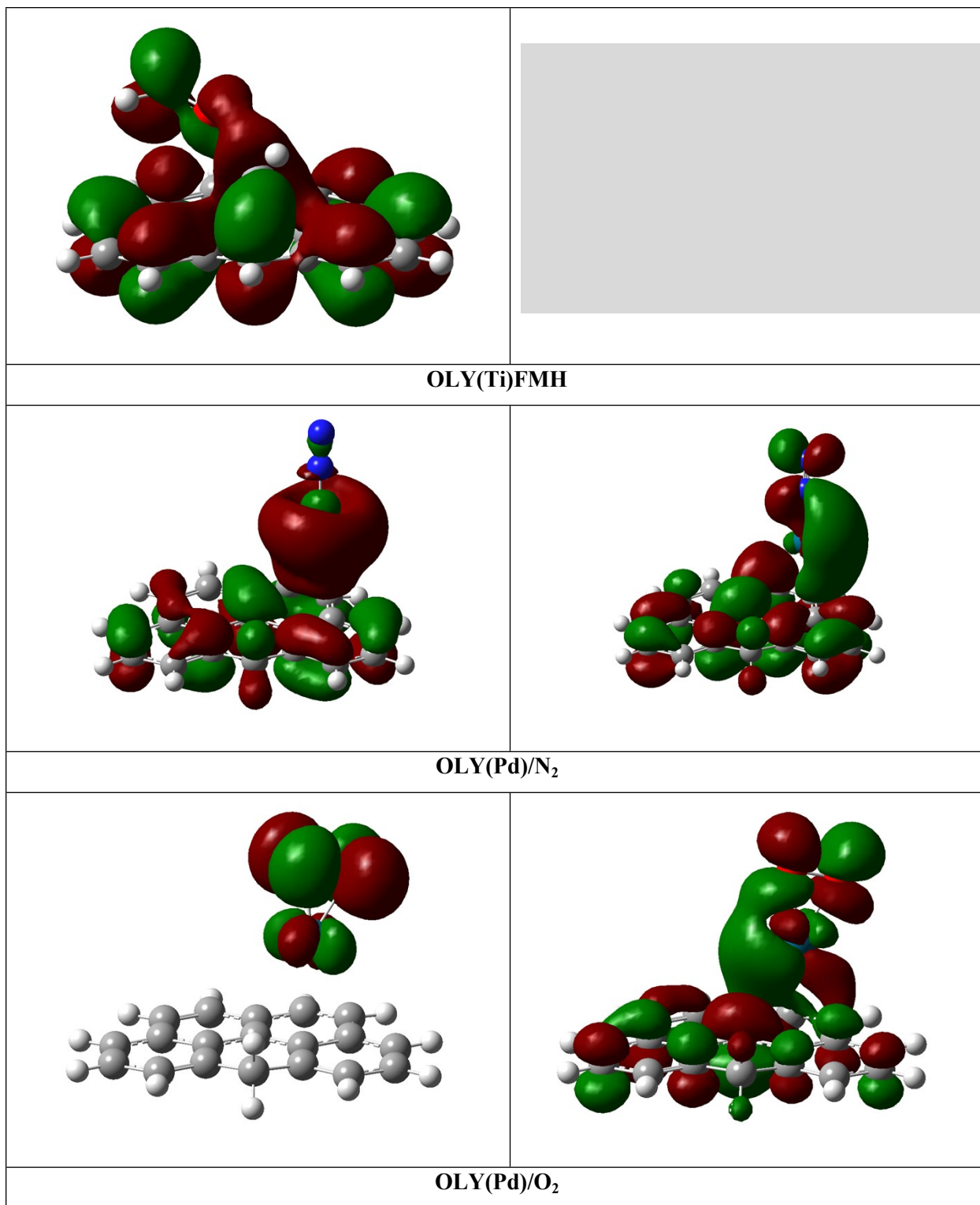
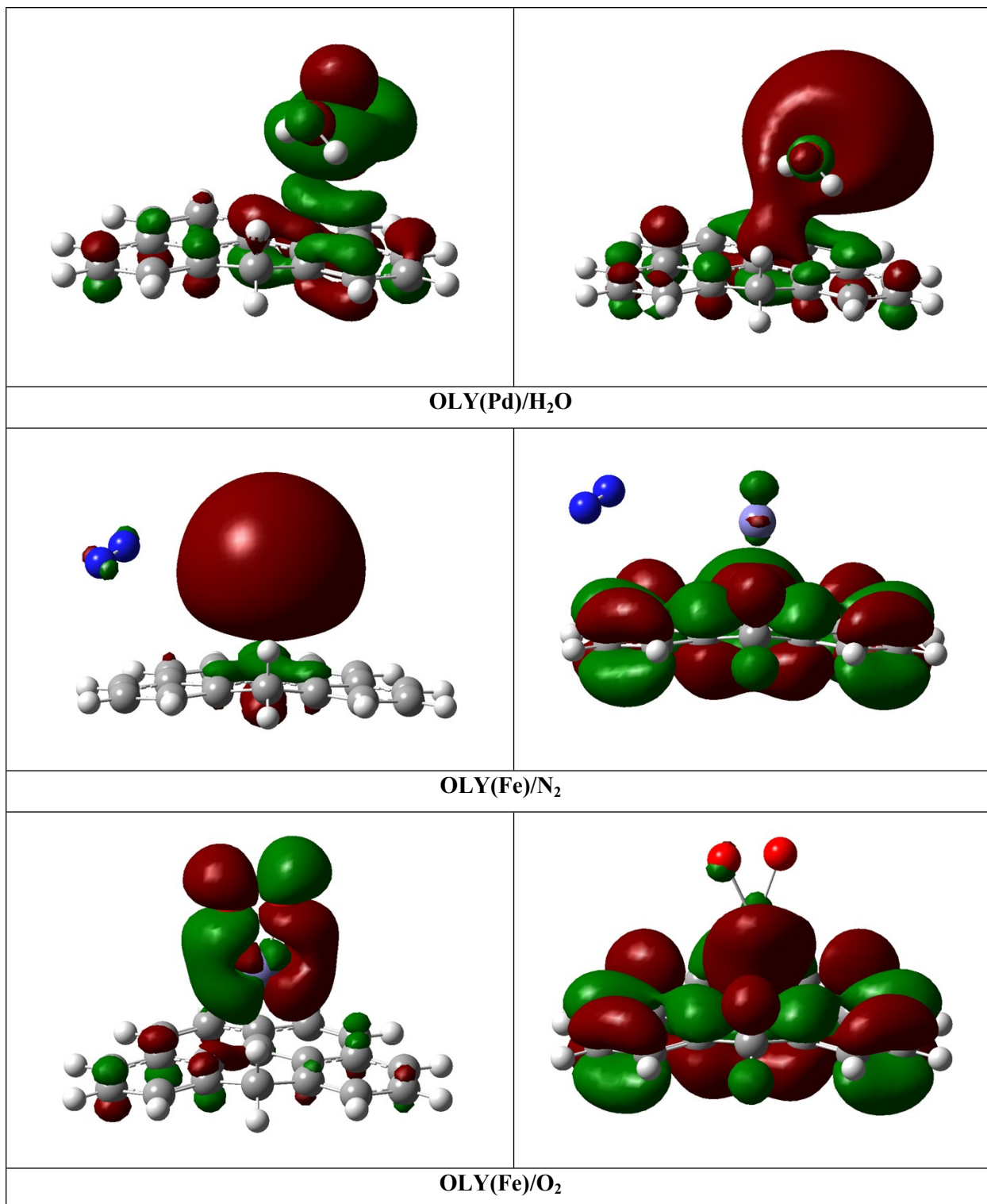
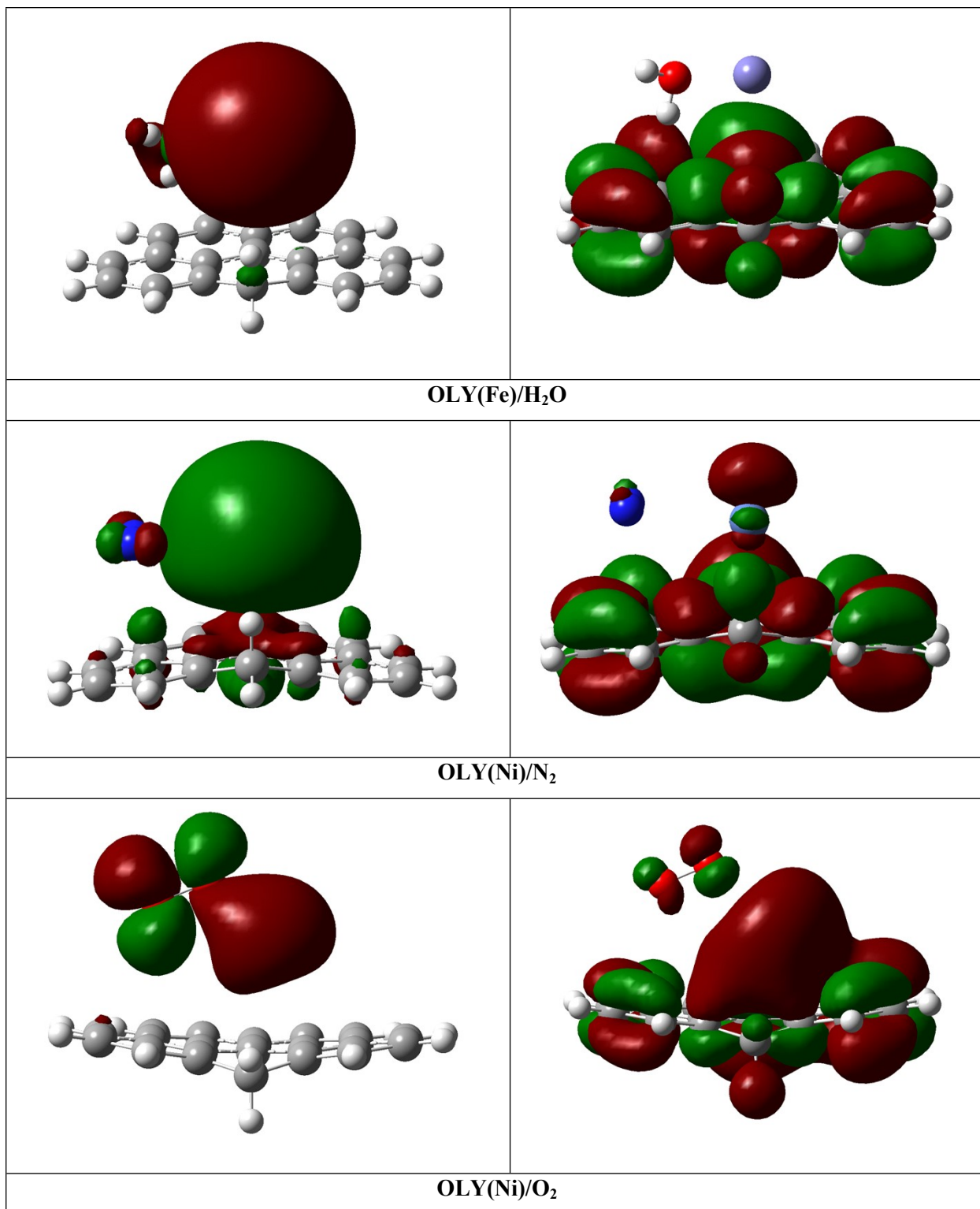


Figure S3: Different orientations are tested to obtain the most stable configuration.









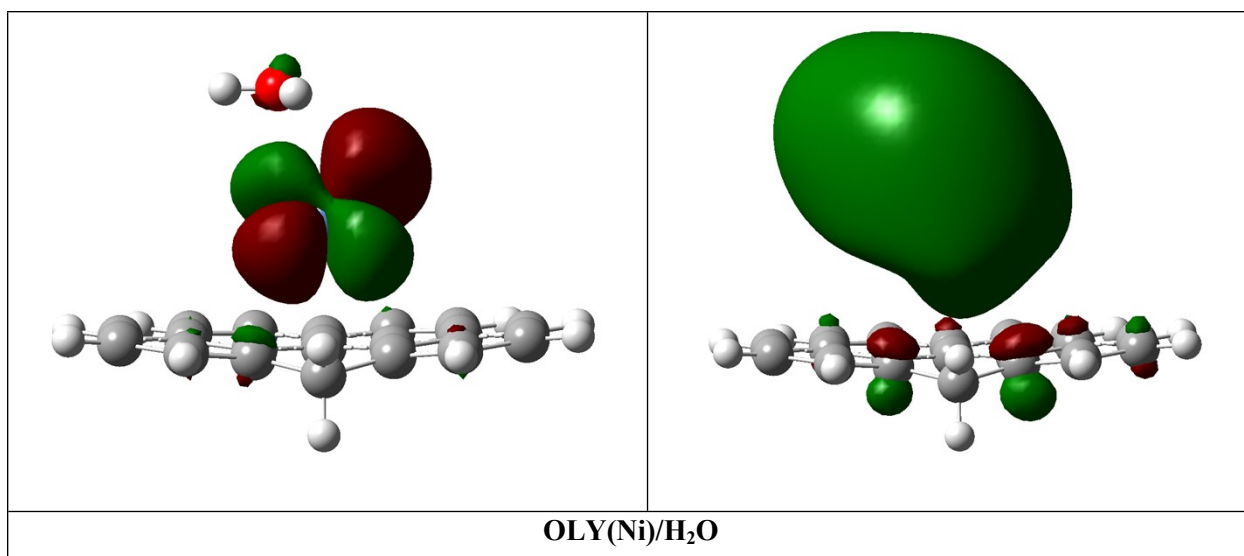
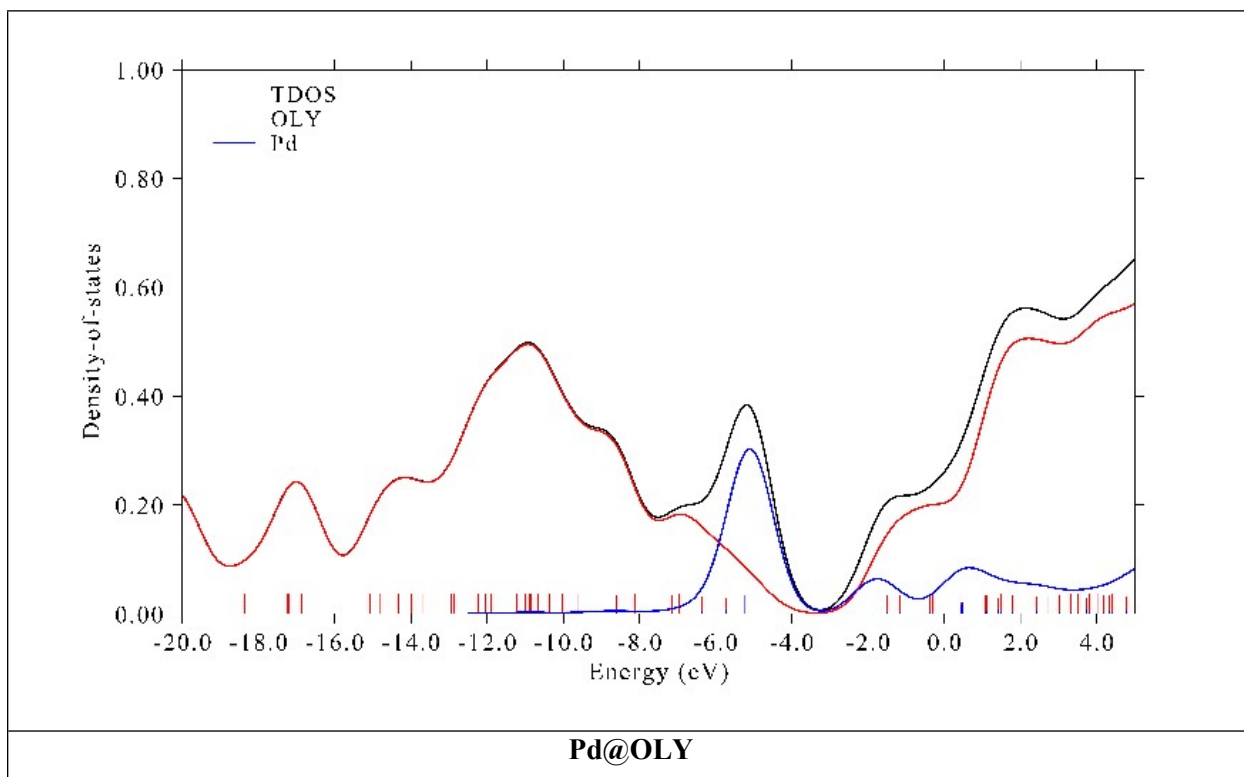
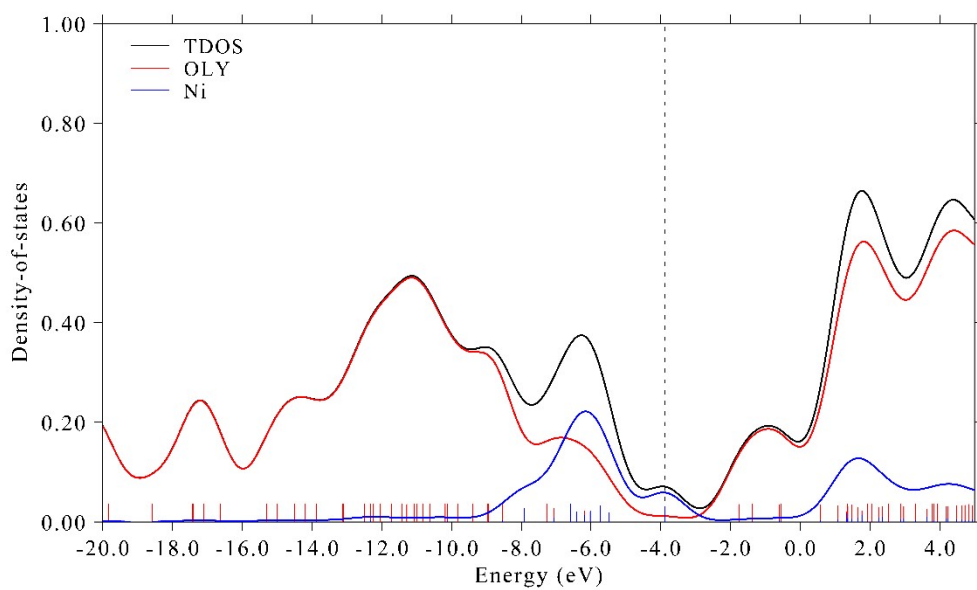
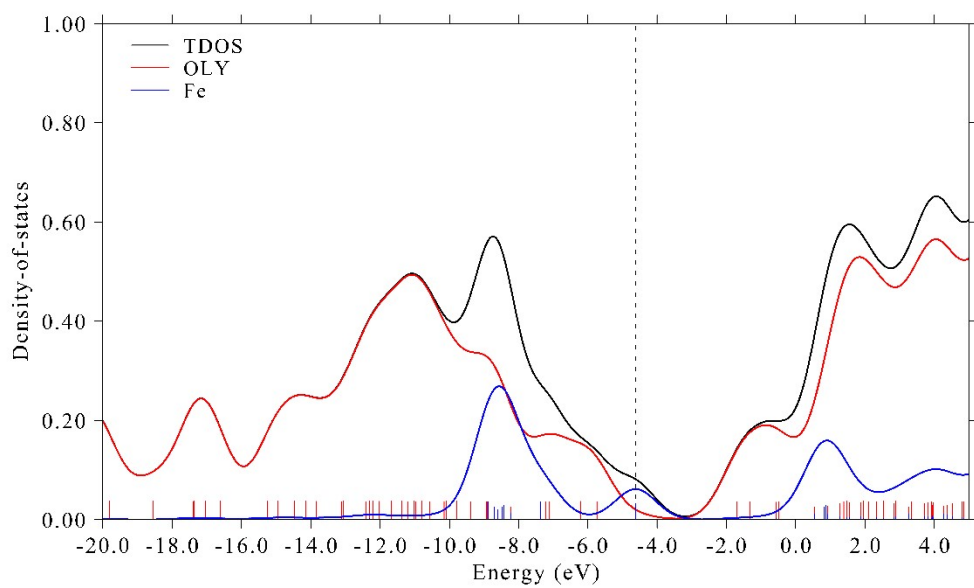


Figure S5: HOMO-LUMO orbital densities of Ti@OLY, OLY(TM)H₂, OLY(TM)O₂, and OLY(TM)H₂O

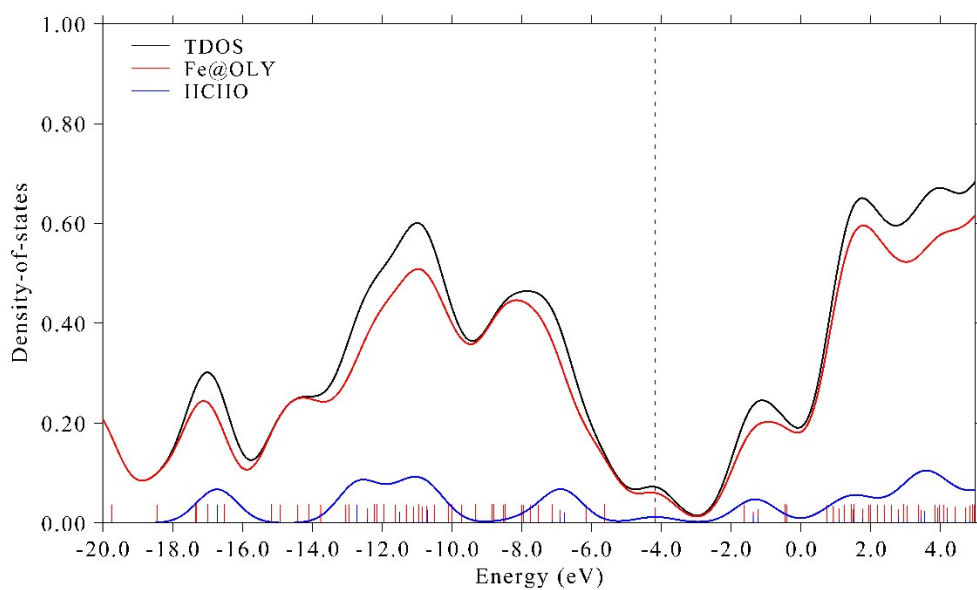




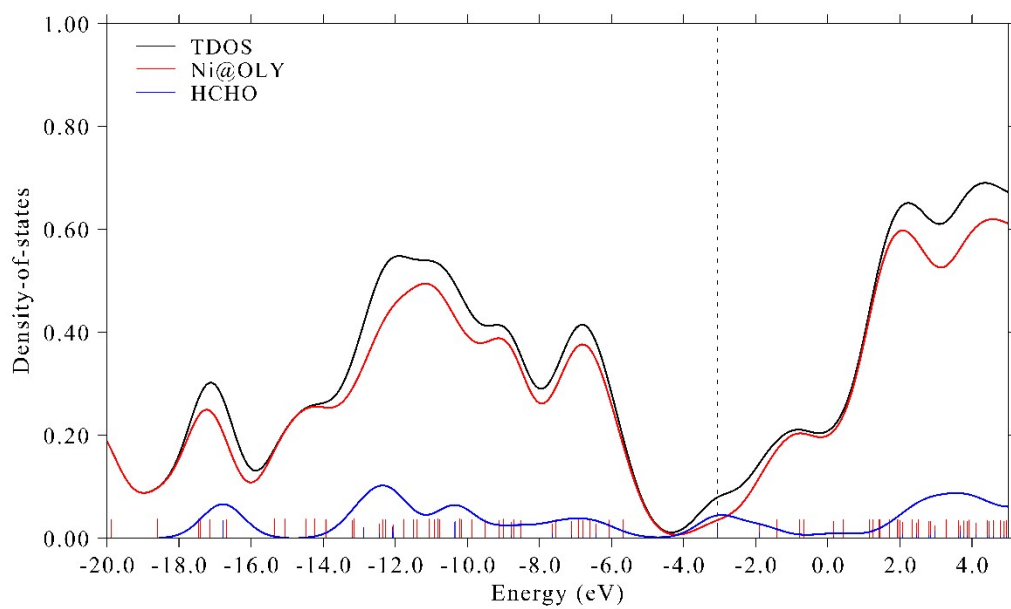
Ni@OLY



Fe@OLY



OLY(Fe)/HCHO



OLY(Ni)/HCHO

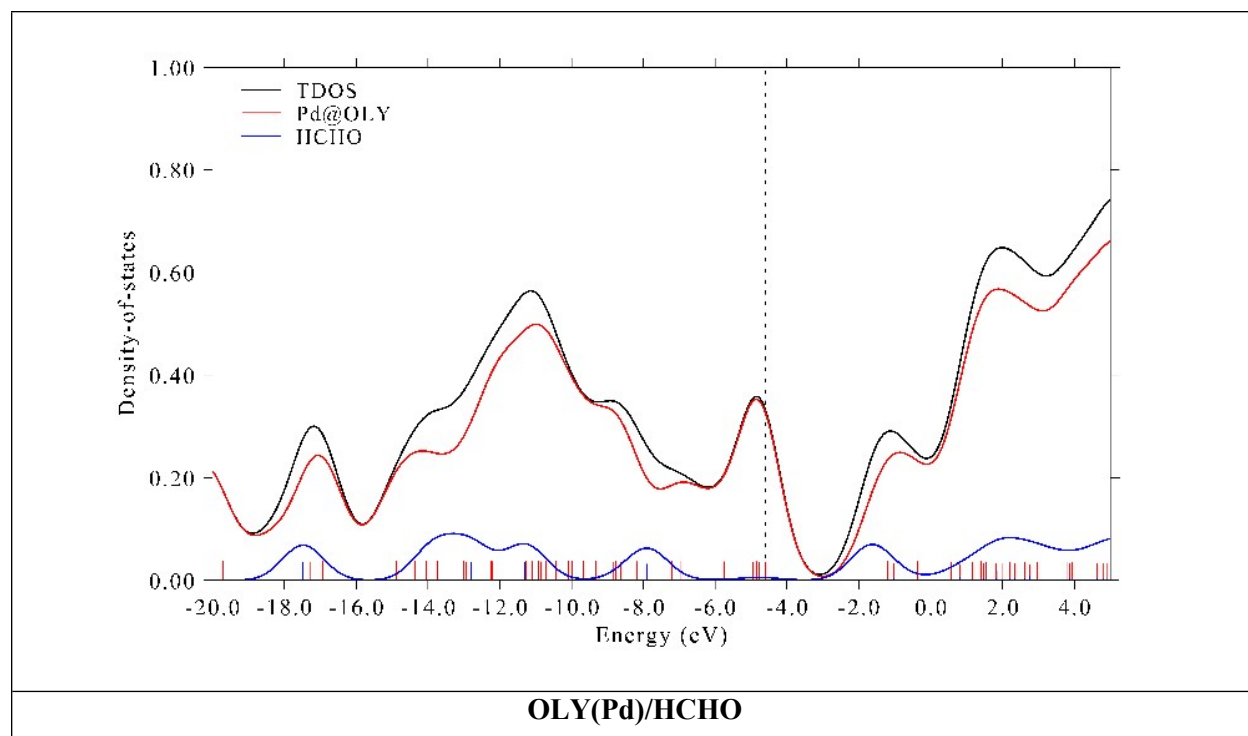


Figure S6: DOS spectra of TM@OLY and OLY(TM)HCHO

Table S4: Recovery time at different temperatures (298K, 350K, and 400K)

Complex (OLY(TM)/HCHO)	Temperature (K)	Recovery time of sensor (s)
OLY(Ni)/HCHO	298	8.9×10^{-1}
	350	2.1×10^{-3}
	400	1.4×10^{-4}
OLY(Fe)/HCHO	298	7.7×10^{-4}
	350	3.7×10^{-5}
	400	4.2×10^{-6}
OLY(Pd)/HCHO	298	1.8×10^{-5}
	350	1.5×10^{-6}
	400	2.5×10^{-7}

Optimized cartesian Coordinates

TM@OLY

Pd@OLY				
xyz 0, 1				
1	C	0.01895	-0.5482	-0.0211
2	C	-1.2349	0.17304	-0.0233
3	C	1.27037	0.16365	-0.0335
4	C	0.02436	2.38627	-0.0972
5	C	-1.2596	1.59064	-0.0519
6	C	1.30453	1.58435	-0.0578
7	C	0.02082	-1.9589	0.00671
8	C	-2.4687	-0.5483	0.01083
9	C	2.50006	-0.5676	-0.0166
10	C	-2.482	2.25412	-0.0476
11	C	2.52997	2.23682	-0.0561
12	C	-1.2305	-2.6767	0.0278
13	C	1.26454	-2.6657	0.01042
14	C	-2.4424	-1.9898	0.03712
15	C	2.45753	-1.9979	0.0015
16	C	-3.6905	0.16139	0.00432
17	C	3.72788	0.13686	-0.019
18	C	-3.6964	1.54534	-0.0223
19	C	3.74213	1.51896	-0.0365
20	H	0.02296	3.00534	-1.0132
21	H	0.02706	3.11123	0.73632
22	H	-2.4952	3.34787	-0.0675
23	H	2.55278	3.33056	-0.0726
24	H	-1.2122	-3.7631	-0.094
25	H	1.24094	-3.7583	0.03021
26	H	-3.3856	-2.5321	-0.0647
27	H	3.40159	-2.5489	0.01008
28	H	-4.6282	-0.3994	0.02892
29	H	4.66217	-0.4305	-0.006
30	H	-4.6438	2.09003	-0.023
31	H	4.69153	2.06023	-0.0365
32	Pd	-1.8402	-2.5883	2.42988

Ni@OLY				
xyz 0,3				

1	C	-0.000352466	-0.578641602	-0.115810538
2	C	-1.248367528	0.149904238	-0.042967459
3	C	1.247496305	0.150114119	-0.042272594
4	C	-0.000514273	2.319056357	-0.432085737
5	C	-1.266236435	1.576388596	-0.081035414
6	C	1.265804403	1.57628006	-0.082798195
7	C	-0.000372838	-2.000202569	-0.135999668
8	C	-2.475443197	-0.580440576	0.052908171
9	C	2.474217403	-0.580101102	0.055149444
10	C	-2.470289936	2.234201579	0.085638202
11	C	2.469739249	2.234225401	0.082530628
12	C	-1.249436485	-2.675968438	-0.133505457
13	C	1.248696297	-2.675947336	-0.130843464
14	C	-2.432115642	-2.000036868	-0.031476364
15	C	2.431097997	-1.999875997	-0.027573686
16	C	-3.675394467	0.142639577	0.197228789
17	C	3.674359533	0.142852362	0.199005576
18	C	-3.669861776	1.519346862	0.231758511
19	C	3.669208353	1.519526259	0.230689724
20	H	-0.001077753	2.502522844	-1.516302604
21	H	-0.000296034	3.303556686	0.039159381
22	H	-2.488073039	3.317697819	0.08350543
23	H	2.487651335	3.317714546	0.078343595
24	H	-1.247883924	-3.758499909	-0.183761044
25	H	1.24726984	-3.758512092	-0.180474851
26	H	-3.367975855	-2.544715499	-0.001237325
27	H	3.366985116	-2.54441054	0.004311455
28	H	-4.608159837	-0.402961144	0.274551943
29	H	4.606913711	-0.402894018	0.277819542
30	H	-4.599495116	2.060125052	0.35542422
31	H	4.598897945	2.060379045	0.353607815
32	Ni	-0.008249176	0.213569667	1.679689281

Fe@OLY				
xyz 0,5				
1	C	0.001858218	-0.609615884	-0.241083123
2	C	-1.230526194	0.121809431	-0.13855602
3	C	1.234893761	0.121575868	-0.139522791
4	C	0.001974768	2.273333663	-0.653467856
5	C	-1.209659177	1.560875341	-0.101383072
6	C	1.215198222	1.560047965	-0.104912958
7	C	0.001736099	-2.031357855	-0.22877779
8	C	-2.468203371	-0.598184827	0.04589027
9	C	2.471955099	-0.598859175	0.045304026
10	C	-2.411511341	2.237327818	0.19987202
11	C	2.416819028	2.236415469	0.194690913
12	C	-1.249420483	-2.695730487	-0.189113085
13	C	1.252463115	-2.696069285	-0.187710493
14	C	-2.432000718	-2.017338363	-0.053439552
15	C	2.435347865	-2.017997092	-0.052016023
16	C	-3.619688097	0.139328189	0.314776468
17	C	3.624422058	0.138546406	0.311709332
18	C	-3.582238845	1.53358738	0.417024977
19	C	3.58786743	1.532497235	0.411601687
20	H	0.001159388	2.264751117	-1.753387144
21	H	0.002783984	3.31812213	-0.339285244
22	H	-2.410935465	3.320110141	0.225955407
23	H	2.416605359	3.319212619	0.219288622
24	H	-1.256011261	-3.779203899	-0.227426399
25	H	1.258699508	-3.779572152	-0.225379371
26	H	-3.365833518	-2.561998047	0.012999929
27	H	3.3689755	-2.562854125	0.015389719
28	H	-4.560065311	-0.383573901	0.441577968
29	H	4.564546753	-0.384836489	0.438397803
30	H	-4.493766952	2.072042392	0.644400283
31	H	4.499848098	2.071045884	0.636927261

32	Fe	-0.00287691	0.688037329	1.391646345
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OLY(TM)FMH

OLY(Fe)FMH				
xyz 0,5				
1	C	0.068105851	-0.684955438	0.0129
2	C	-1.147897813	0.091151639	0.05117
3	C	1.352251494	-0.02949654	0.02487
4	C	0.210795654	2.217344456	0.31958
5	C	-1.104096953	1.500466736	0.15818
6	C	1.445332215	1.375717795	0.13384
7	C	4.16991E-05	-2.090577111	-0.083
8	C	-2.402573967	-0.57606358	-0.0237
9	C	2.536870373	-0.814831936	-0.0644
10	C	-2.288839549	2.208880432	0.15967
11	C	2.692811192	1.967247042	0.14389
12	C	-1.276382072	-2.724107185	-0.136
13	C	1.208862268	-2.844509994	-0.1589
14	C	-2.425578453	-1.999592781	-0.1158
15	C	2.422333958	-2.233756032	-0.1576
16	C	-3.585278656	0.185198134	-0.0037
17	C	3.788003858	-0.168729802	-0.0463
18	C	-3.526355912	1.556691072	0.07995
19	C	3.86277551	1.20049886	0.05429
20	H	0.246299987	3.077249961	-0.3551
21	H	0.258146099	2.639059067	1.33053
22	H	-2.258577064	3.289127822	0.23862
23	H	2.764938641	3.041688286	0.25334
24	H	-1.311050378	-3.804558829	-0.2013
25	H	1.138071067	-3.923088362	-0.2257
26	H	-3.386537341	-2.496758226	-0.1627
27	H	3.330896803	-2.82013551	-0.2188

28	H	-4.539129163	-0.324370408	-0.0582
29	H	4.68935103	-0.763957528	-0.1098
30	H	-4.43837418	2.13951996	0.09035
31	H	4.828363777	1.690374637	0.07575
32	Fe	0.019836628	-0.656464433	2.58503
33	C	1.920256145	1.327698996	3.51484
34	H	2.581051855	0.696921248	2.89115
35	H	1.630818844	0.90052213	4.49124
36	O	1.621472634	2.46421706	3.20099

OLY(Ni)FMH				
xyz 0,3				
1	C	0.00023751	-0.57356796	-0.16507724
2	C	-1.24515	0.14329838	-0.10692195
3	C	1.24697695	0.14264204	-0.1140374
4	C	0.0005888	2.33090441	-0.35750654
5	C	-1.27020001	1.56127024	-0.10385295
6	C	1.27023581	1.55970277	-0.10317092
7	C	0.00047061	-1.97918896	-0.15615674
8	C	-2.46496538	-0.58272925	-0.01047576
9	C	2.46650211	-0.58274426	-0.01843184
10	C	-2.47652785	2.21571035	0.04009702
11	C	2.47590278	2.21434444	0.05069209
12	C	-1.2418003	-2.67503743	-0.1195507
13	C	1.24392252	-2.67481937	-0.1255472
14	C	-2.42310482	-2.00652969	-0.03935578
15	C	2.42528428	-2.00720443	-0.04990187
16	C	-3.67373074	0.12644639	0.12404614
17	C	3.67463561	0.12601496	0.11974784
18	C	-3.67646678	1.50122505	0.16081921
19	C	3.67619606	1.50068975	0.16732777
20	H	0.00180798	2.63645679	-1.41296355
21	H	0.00093241	3.2557725	0.22189445

22	H	-2.49413109	3.29882087	0.05771426
23	H	2.49209661	3.29735091	0.07561831
24	H	-1.22595711	-3.75807719	-0.12690842
25	H	1.22749556	-3.75788027	-0.13395963
26	H	-3.35794037	-2.550662	0.01640506
27	H	3.3604929	-2.55093744	0.00276906
28	H	-4.60057025	-0.42794084	0.20441869
29	H	4.60186699	-0.42803136	0.19778223
30	H	-4.60861866	2.03879702	0.27793355
31	H	4.60767912	2.03811097	0.29023314
32	Ni	-0.03541953	0.40468599	2.27949698
33	C	1.91536878	-0.16086882	4.27742575
34	H	2.84968421	-0.69777954	4.5351101
35	H	1.78520719	0.83514238	4.74482333
36	O	1.09517957	-0.62855565	3.53815566

OLY(Pd)FMH				
xyz 0,1				
1	C	0.02186896	-0.54415755	-0.02541241
2	C	-1.22690491	0.17286395	-0.02416714
3	C	1.26725972	0.16521707	-0.03727471
4	C	0.02532284	2.37857872	-0.1047975
5	C	-1.25416295	1.58283942	-0.05093547
6	C	1.30208727	1.57829723	-0.05997368
7	C	0.02504423	-1.94646048	0.00467457
8	C	-2.45350574	-0.54562903	0.01286689
9	C	2.49063573	-0.56254083	-0.01951751
10	C	-2.46989443	2.2409865	-0.04087994
11	C	2.52026356	2.22670395	-0.05452345
12	C	-1.21933263	-2.66095999	0.0284453
13	C	1.26303842	-2.64986848	0.00597587
14	C	-2.42555816	-1.98042486	0.03661613
15	C	2.44850532	-1.98643219	-0.00332262

16	C	-3.66998396	0.15851231	0.0090887
17	C	3.71222148	0.13805016	-0.01918624
18	C	-3.67759447	1.53428237	-0.01435121
19	C	3.72634384	1.51220638	-0.03400629
20	H	0.02255788	2.98151215	-1.01991416
21	H	0.02874801	3.10326213	0.71584851
22	H	-2.48626191	3.32480221	-0.05862937
23	H	2.54429802	3.31053109	-0.06914007
24	H	-1.20111943	-3.73821431	-0.08198146
25	H	1.23922713	-3.73266287	0.02617361
26	H	-3.35884219	-2.52012298	-0.0637491
27	H	3.38448457	-2.53165347	0.00421448
28	H	-4.59815495	-0.39886279	0.03573334
29	H	4.63842173	-0.42339709	-0.00567784
30	H	-4.61590139	2.07413387	-0.01164022
31	H	4.66685215	2.048246	-0.03126984
32	Pd	-1.920121	-2.58660707	2.42443556
33	C	1.0285012	-1.42210947	4.82553778
34	H	2.02072706	-1.15538333	4.41085153
35	H	0.94006097	-1.3863537	5.9293225
36	O	0.10669902	-1.73055391	4.12332388

Vibrational Frequencies for all stable geometries

Pd@OLY		
0	0	cm ⁻¹
1	0	cm ⁻¹
2	0	cm ⁻¹
3	0	cm ⁻¹
4	0	cm ⁻¹
5	0	cm ⁻¹
6	7.66	cm ⁻¹
7	33.09	cm ⁻¹
8	38.08	cm ⁻¹

9	83.76	cm**-1
10	171.67	cm**-1
11	183.38	cm**-1
12	202.31	cm**-1
13	276.02	cm**-1
14	282.86	cm**-1
15	307.76	cm**-1
16	392.39	cm**-1
17	393.94	cm**-1
18	444.11	cm**-1
19	446.79	cm**-1
20	450.16	cm**-1
21	503.28	cm**-1
22	514.58	cm**-1
23	528.12	cm**-1
24	538.25	cm**-1
25	554.45	cm**-1
26	568.82	cm**-1
27	584.87	cm**-1
28	597.03	cm**-1
29	609.33	cm**-1
30	647.88	cm**-1
31	679.7	cm**-1
32	700.13	cm**-1
33	763.46	cm**-1
34	764.31	cm**-1
35	773.31	cm**-1
36	775.88	cm**-1
37	793.52	cm**-1
38	816.55	cm**-1
39	826.89	cm**-1
40	833.94	cm**-1
41	851.02	cm**-1
42	895.9	cm**-1
43	902.41	cm**-1
44	934.46	cm**-1
45	947.09	cm**-1
46	949.2	cm**-1
47	951.73	cm**-1
48	954.58	cm**-1
49	964.55	cm**-1

50	969.59	cm**-1
51	1039.78	cm**-1
52	1083.13	cm**-1
53	1112.04	cm**-1
54	1117.38	cm**-1
55	1157.78	cm**-1
56	1174.03	cm**-1
57	1192.2	cm**-1
58	1194.04	cm**-1
59	1210.97	cm**-1
60	1237.05	cm**-1
61	1239	cm**-1
62	1246.47	cm**-1
63	1262	cm**-1
64	1273.81	cm**-1
65	1306.88	cm**-1
66	1316.32	cm**-1
67	1368.44	cm**-1
68	1377.47	cm**-1
69	1413.56	cm**-1
70	1418.42	cm**-1
71	1429.8	cm**-1
72	1448.86	cm**-1
73	1458.48	cm**-1
74	1469.22	cm**-1
75	1493.41	cm**-1
76	1518.82	cm**-1
77	1534.56	cm**-1
78	1557.69	cm**-1
79	1617.15	cm**-1
80	1622.37	cm**-1
81	1638.11	cm**-1
82	1643.98	cm**-1
83	1658	cm**-1
84	3003.71	cm**-1
85	3023.29	cm**-1
86	3154.97	cm**-1
87	3156.02	cm**-1
88	3160.42	cm**-1
89	3162.42	cm**-1
90	3167.42	cm**-1

91	3168.66	cm**-1
92	3176.98	cm**-1
93	3179.86	cm**-1
94	3186.57	cm**-1
95	3187.13	cm**-1

OLY(Pd)FMH		
0	0	cm**-1
1	0	cm**-1
2	0	cm**-1
3	0	cm**-1
4	0	cm**-1
5	0	cm**-1
6	6.8	cm**-1
7	23.03	cm**-1
8	35.92	cm**-1
9	40.58	cm**-1
10	58.21	cm**-1
11	67.76	cm**-1
12	87.88	cm**-1
13	98.56	cm**-1
14	150.93	cm**-1
15	172.09	cm**-1
16	183.53	cm**-1
17	196.21	cm**-1
18	205.23	cm**-1
19	277.76	cm**-1
20	291.73	cm**-1
21	310.16	cm**-1
22	393.43	cm**-1
23	395.07	cm**-1
24	445.4	cm**-1
25	447.98	cm**-1
26	452.59	cm**-1
27	507.77	cm**-1
28	518.79	cm**-1
29	527.95	cm**-1
30	539.12	cm**-1
31	552.39	cm**-1

32	566.32	cm**-1
33	583.71	cm**-1
34	601.6	cm**-1
35	611.2	cm**-1
36	649.52	cm**-1
37	683.2	cm**-1
38	703.32	cm**-1
39	763.71	cm**-1
40	764.37	cm**-1
41	775.9	cm**-1
42	778.11	cm**-1
43	793.79	cm**-1
44	813.39	cm**-1
45	833.15	cm**-1
46	839.87	cm**-1
47	853.14	cm**-1
48	896.29	cm**-1
49	904.73	cm**-1
50	937.95	cm**-1
51	951.16	cm**-1
52	952.95	cm**-1
53	954.12	cm**-1
54	965.45	cm**-1
55	970.42	cm**-1
56	976.3	cm**-1
57	1039.62	cm**-1
58	1082.72	cm**-1
59	1110.24	cm**-1
60	1118.04	cm**-1
61	1159.88	cm**-1
62	1173.61	cm**-1
63	1192.12	cm**-1
64	1193.54	cm**-1
65	1198.65	cm**-1
66	1210.97	cm**-1
67	1232.06	cm**-1
68	1237.19	cm**-1
69	1251.33	cm**-1
70	1261.84	cm**-1
71	1263.41	cm**-1
72	1273.65	cm**-1

73	1307.05	cm** ⁻¹
74	1315.85	cm** ⁻¹
75	1368.83	cm** ⁻¹
76	1377.82	cm** ⁻¹
77	1412.47	cm** ⁻¹
78	1417.96	cm** ⁻¹
79	1429.77	cm** ⁻¹
80	1449.53	cm** ⁻¹
81	1459.32	cm** ⁻¹
82	1468.9	cm** ⁻¹
83	1491.68	cm** ⁻¹
84	1518.12	cm** ⁻¹
85	1522.9	cm** ⁻¹
86	1534.05	cm** ⁻¹
87	1554.97	cm** ⁻¹
88	1617.96	cm** ⁻¹
89	1621.45	cm** ⁻¹
90	1638.04	cm** ⁻¹
91	1642.01	cm** ⁻¹
92	1655.17	cm** ⁻¹
93	1771.1	cm** ⁻¹
94	2920.54	cm** ⁻¹
95	2977.65	cm** ⁻¹
96	3025.97	cm** ⁻¹
97	3046.89	cm** ⁻¹
98	3156.93	cm** ⁻¹
99	3157.49	cm** ⁻¹
100	3161.25	cm** ⁻¹
101	3166.13	cm** ⁻¹
102	3166.71	cm** ⁻¹
103	3169.46	cm** ⁻¹
104	3179.45	cm** ⁻¹
105	3182.9	cm** ⁻¹
106	3186.44	cm** ⁻¹
107	3187.21	cm** ⁻¹

Ni@OLY		
0	0	cm** ⁻¹
1	0	cm** ⁻¹
2	0	cm** ⁻¹
3	0	cm** ⁻¹

4	0	cm**-1
5	0	cm**-1
6	7.79	cm**-1
7	11.19	cm**-1
8	64.83	cm**-1
9	92.29	cm**-1
10	93.13	cm**-1
11	179.46	cm**-1
12	207.54	cm**-1
13	210.67	cm**-1
14	276.46	cm**-1
15	281.3	cm**-1
16	313.19	cm**-1
17	392.32	cm**-1
18	398.31	cm**-1
19	430.84	cm**-1
20	440.01	cm**-1
21	450.58	cm**-1
22	510.1	cm**-1
23	519.6	cm**-1
24	520.05	cm**-1
25	530.36	cm**-1
26	566.65	cm**-1
27	582.2	cm**-1
28	594.22	cm**-1
29	596.47	cm**-1
30	648.87	cm**-1
31	677.88	cm**-1
32	704.57	cm**-1
33	755.2	cm**-1
34	764.53	cm**-1
35	766.21	cm**-1
36	775.6	cm**-1
37	795.19	cm**-1
38	809.47	cm**-1
39	832.24	cm**-1
40	833.18	cm**-1
41	851.35	cm**-1
42	897.47	cm**-1
43	905.02	cm**-1
44	949.27	cm**-1

45	950.47	cm**-1
46	953.39	cm**-1
47	958.64	cm**-1
48	962.14	cm**-1
49	963.98	cm**-1
50	973.1	cm**-1
51	1040.83	cm**-1
52	1083.43	cm**-1
53	1110.02	cm**-1
54	1121.11	cm**-1
55	1170.93	cm**-1
56	1174.78	cm**-1
57	1194.28	cm**-1
58	1196.18	cm**-1
59	1212.36	cm**-1
60	1232.17	cm**-1
61	1242.21	cm**-1
62	1256.83	cm**-1
63	1263.35	cm**-1
64	1276.5	cm**-1
65	1310.47	cm**-1
66	1313.86	cm**-1
67	1375.31	cm**-1
68	1378.47	cm**-1
69	1416.62	cm**-1
70	1417.1	cm**-1
71	1430.59	cm**-1
72	1456.74	cm**-1
73	1459.42	cm**-1
74	1471.04	cm**-1
75	1486.86	cm**-1
76	1525.12	cm**-1
77	1540.06	cm**-1
78	1554.48	cm**-1
79	1618.06	cm**-1
80	1638.69	cm**-1
81	1640.96	cm**-1
82	1641.77	cm**-1
83	1664.33	cm**-1
84	2973.15	cm**-1
85	3064.88	cm**-1

86	3162.32	cm**-1
87	3163	cm**-1
88	3163.18	cm**-1
89	3164.57	cm**-1
90	3171.33	cm**-1
91	3171.62	cm**-1
92	3180.42	cm**-1
93	3182.13	cm**-1
94	3189.16	cm**-1
95	3189.46	cm**-1

OLY(Ni)FMH		
0	0	cm**-1
1	0	cm**-1
2	0	cm**-1
3	0	cm**-1
4	0	cm**-1
5	0	cm**-1
6	40.76	cm**-1
7	45.83	cm**-1
8	67.71	cm**-1
9	73.16	cm**-1
10	97.34	cm**-1
11	102.51	cm**-1
12	145.39	cm**-1
13	161.91	cm**-1
14	198.11	cm**-1
15	212.65	cm**-1
16	225.35	cm**-1
17	238.4	cm**-1
18	281.59	cm**-1
19	287.35	cm**-1
20	309.86	cm**-1
21	325.62	cm**-1
22	389.51	cm**-1
23	401.2	cm**-1
24	427.77	cm**-1
25	446.21	cm**-1
26	452.55	cm**-1
27	490.28	cm**-1
28	513.35	cm**-1

29	518.98	cm**-1
30	527.26	cm**-1
31	533.5	cm**-1
32	560.22	cm**-1
33	573.24	cm**-1
34	591.82	cm**-1
35	595.99	cm**-1
36	598.31	cm**-1
37	641.49	cm**-1
38	676.5	cm**-1
39	703.33	cm**-1
40	753.53	cm**-1
41	759.11	cm**-1
42	759.63	cm**-1
43	768.55	cm**-1
44	784.81	cm**-1
45	803.1	cm**-1
46	820.91	cm**-1
47	829.32	cm**-1
48	843.24	cm**-1
49	887.93	cm**-1
50	895.28	cm**-1
51	940.04	cm**-1
52	940.84	cm**-1
53	946.95	cm**-1
54	950.87	cm**-1
55	956.38	cm**-1
56	967.55	cm**-1
57	972.87	cm**-1
58	1031.37	cm**-1
59	1078.7	cm**-1
60	1102.55	cm**-1
61	1118.93	cm**-1
62	1164.59	cm**-1
63	1168.29	cm**-1
64	1186	cm**-1
65	1190.81	cm**-1
66	1192.1	cm**-1
67	1199.51	cm**-1
68	1221.36	cm**-1
69	1234.79	cm**-1

70	1243.39	cm**-1
71	1255.28	cm**-1
72	1261.52	cm**-1
73	1271.62	cm**-1
74	1301.87	cm**-1
75	1304.59	cm**-1
76	1366.93	cm**-1
77	1370.87	cm**-1
78	1397.14	cm**-1
79	1411.63	cm**-1
80	1424.82	cm**-1
81	1448.97	cm**-1
82	1453.93	cm**-1
83	1462.93	cm**-1
84	1481.19	cm**-1
85	1510.87	cm**-1
86	1513.71	cm**-1
87	1527.93	cm**-1
88	1539.3	cm**-1
89	1593.74	cm**-1
90	1599.11	cm**-1
91	1613.78	cm**-1
92	1625.74	cm**-1
93	1639.56	cm**-1
94	2937.57	cm**-1
95	3060.23	cm**-1
96	3068.67	cm**-1
97	3161.89	cm**-1
98	3163.9	cm**-1
99	3165.47	cm**-1
100	3165.79	cm**-1
101	3169.18	cm**-1
102	3173.27	cm**-1
103	3173.91	cm**-1
104	3180.05	cm**-1
105	3181.47	cm**-1
106	3189.54	cm**-1
107	3190.02	cm**-1

Fe@OLY		
0	0	cm**-1

1	0	cm**-1
2	0	cm**-1
3	0	cm**-1
4	0	cm**-1
5	0	cm**-1
6	13.4	cm**-1
7	34.23	cm**-1
8	51.19	cm**-1
9	61.46	cm**-1
10	93.41	cm**-1
11	174.7	cm**-1
12	191.1	cm**-1
13	212.95	cm**-1
14	283.9	cm**-1
15	284.12	cm**-1
16	309.98	cm**-1
17	393.77	cm**-1
18	395.26	cm**-1
19	436.43	cm**-1
20	438.56	cm**-1
21	450.41	cm**-1
22	508.97	cm**-1
23	518.06	cm**-1
24	528.93	cm**-1
25	534.71	cm**-1
26	566.86	cm**-1
27	583.54	cm**-1
28	599.37	cm**-1
29	601.5	cm**-1
30	648.09	cm**-1
31	678.77	cm**-1
32	703.03	cm**-1
33	764.95	cm**-1
34	766.08	cm**-1
35	770.72	cm**-1
36	778.31	cm**-1
37	797.36	cm**-1
38	815.27	cm**-1
39	832.77	cm**-1
40	838.87	cm**-1
41	854.53	cm**-1

42	901.14	cm**-1
43	908.49	cm**-1
44	952.59	cm**-1
45	956.54	cm**-1
46	957.26	cm**-1
47	962.71	cm**-1
48	967.24	cm**-1
49	969.14	cm**-1
50	975	cm**-1
51	1042.28	cm**-1
52	1083.22	cm**-1
53	1111.76	cm**-1
54	1120.37	cm**-1
55	1171.51	cm**-1
56	1177.04	cm**-1
57	1194.33	cm**-1
58	1197.27	cm**-1
59	1215.62	cm**-1
60	1237.57	cm**-1
61	1240.75	cm**-1
62	1257.13	cm**-1
63	1266.49	cm**-1
64	1277.89	cm**-1
65	1310.49	cm**-1
66	1318.16	cm**-1
67	1376.31	cm**-1
68	1379.31	cm**-1
69	1417.49	cm**-1
70	1419.62	cm**-1
71	1433.66	cm**-1
72	1453.58	cm**-1
73	1458.14	cm**-1
74	1473.13	cm**-1
75	1491.25	cm**-1
76	1525.02	cm**-1
77	1543.3	cm**-1
78	1559.75	cm**-1
79	1622.71	cm**-1
80	1641.99	cm**-1
81	1644.33	cm**-1
82	1644.68	cm**-1

83	1666.13	cm ^{**} -1
84	2978.66	cm ^{**} -1
85	3047.24	cm ^{**} -1
86	3159.74	cm ^{**} -1
87	3160.46	cm ^{**} -1
88	3165.24	cm ^{**} -1
89	3166.77	cm ^{**} -1
90	3171.13	cm ^{**} -1
91	3171.39	cm ^{**} -1
92	3182.61	cm ^{**} -1
93	3184.58	cm ^{**} -1
94	3188.8	cm ^{**} -1
95	3189.37	cm ^{**} -1

OLY(Fe)FMH		
0	0	cm ^{**} -1
1	0	cm ^{**} -1
2	0	cm ^{**} -1
3	0	cm ^{**} -1
4	0	cm ^{**} -1
5	0	cm ^{**} -1
6	24.98	cm ^{**} -1
7	27.33	cm ^{**} -1
8	35.48	cm ^{**} -1
9	50.73	cm ^{**} -1
10	63.93	cm ^{**} -1
11	83.9	cm ^{**} -1
12	93.88	cm ^{**} -1
13	116.18	cm ^{**} -1
14	173.32	cm ^{**} -1
15	188.22	cm ^{**} -1
16	211.93	cm ^{**} -1
17	217.08	cm ^{**} -1
18	282.55	cm ^{**} -1
19	285.45	cm ^{**} -1
20	309.58	cm ^{**} -1
21	393.87	cm ^{**} -1
22	396.43	cm ^{**} -1
23	440.61	cm ^{**} -1

24	444.18	cm**-1
25	444.98	cm**-1
26	450.29	cm**-1
27	497.22	cm**-1
28	512.55	cm**-1
29	517.56	cm**-1
30	529.32	cm**-1
31	538.51	cm**-1
32	567.13	cm**-1
33	583.85	cm**-1
34	600.1	cm**-1
35	606.96	cm**-1
36	649.56	cm**-1
37	678.87	cm**-1
38	703.8	cm**-1
39	763.88	cm**-1
40	766.16	cm**-1
41	770.72	cm**-1
42	776.94	cm**-1
43	797.37	cm**-1
44	816.22	cm**-1
45	830.34	cm**-1
46	837.7	cm**-1
47	854.34	cm**-1
48	896.43	cm**-1
49	904.27	cm**-1
50	952.01	cm**-1
51	952.54	cm**-1
52	957.81	cm**-1
53	959.65	cm**-1
54	967.88	cm**-1
55	968.75	cm**-1
56	974.22	cm**-1
57	993.37	cm**-1
58	1042.54	cm**-1
59	1083.36	cm**-1
60	1112.36	cm**-1
61	1118.91	cm**-1
62	1171.15	cm**-1
63	1175.74	cm**-1
64	1193.86	cm**-1

65	1196.66	cm**-1
66	1213.93	cm**-1
67	1217.23	cm**-1
68	1240.14	cm**-1
69	1247.39	cm**-1
70	1254.25	cm**-1
71	1265.85	cm**-1
72	1277.87	cm**-1
73	1310.84	cm**-1
74	1318.66	cm**-1
75	1374.54	cm**-1
76	1379.51	cm**-1
77	1415.06	cm**-1
78	1420.76	cm**-1
79	1421.83	cm**-1
80	1433.02	cm**-1
81	1447.33	cm**-1
82	1457.34	cm**-1
83	1472.42	cm**-1
84	1491.03	cm**-1
85	1525.4	cm**-1
86	1543.16	cm**-1
87	1559.15	cm**-1
88	1590.15	cm**-1
89	1621.42	cm**-1
90	1640.37	cm**-1
91	1643.31	cm**-1
92	1644.14	cm**-1
93	1666.11	cm**-1
94	2934.69	cm**-1
95	2991.94	cm**-1
96	3000.8	cm**-1
97	3072.72	cm**-1
98	3160.4	cm**-1
99	3162.04	cm**-1
100	3163.18	cm**-1
101	3164.6	cm**-1
102	3169.52	cm**-1
103	3171.96	cm**-1
104	3179.87	cm**-1
105	3182.21	cm**-1

106	3186.88	cm ⁻¹
107	3188.6	cm ⁻¹