

Table S1: Calculated catalyst Descriptors																		
S/NO.	Catalyst	Total K.E	Total P.E	Hamiltonian	CO2 S.P.E	Average B.E	Atomic No	Group	covalent radius	Bond length	surface free energy	work function	partial electronegativity	enthalpy of fusion	density	wigner seitz radius	Period	atomic mass
1	Ni	1.6	-10.18	-10.18	-0.43	-9.75	28	10	124	2.956	1.22	4.3	1.91	-1122.27	8.908	124	4	58.693
2	Cu	0.92	-8.92	-8.92	-0.37	-8.7	29	11	132	3.577	1.44	4.4	1.9	-107.18	8.96	128	4	63.546
3	C	3.13	-5.05	-5.05	2.69	-7.75	6	14	76	6.054	2.52	4.6	2.55	200.73	2.26	77	2	12.011
4	Pb	0.67	-3.2	-3.2	3.16	-6.67	82	14	146	3.684	0.27	4	2.33	-86.84	11.34	147	6	207.2
5	Al	0.5	-2.82	-2.82	3.16	-6.17	13	13	121	3.754	0.82	4.25	1.61	-76.99	2.7	118	3	26.982
6	In	2.06	-2.55	-2.55	3.12	-5.89	49	13	142	4.023	0.38	3.8	1.78	-18.93	7.31	156	6	114.9
7	Cd	3.13	-2.1	-2.1	3.15	-5.43	48	12	144	3.193	0.21	4.1	1.69	-36.4	8.65	144	5	112.4
8	Pd	2.11	-1.55	-1.55	3.59	-5.14	46	10	146	3.184	1.51	5.12	2.2	-7.3764	12.023	137	5	106.4
9	Ir	3.13	-1.2	-1.2	3.23	-5.08	77	9	141	2.974	2.84	5.27	2.2	156.26	22.56	135	6	192.2
10	Be	1.69	-1.71	-1.71	3.17	-4.89	4	2	96	3.279	1.77	3.92	1.57	-7.63	1.848	112	2	9.012
11	Si	2.19	-4.84	-4.84	-0.04	-4.81	14	14	111	3.884	NA	4.2	1.9	-238.14	2.33	117	3	28.09
12	Au	1.13	-1.35	-1.35	3.39	-4.74	79	11	136	3.245	0.86	4.3	2.54	-5.503	19.3	144	6	196.97
13	Ag	2.16	-1.31	-1.31	3.21	-4.44	47	11	145	3.809	0.84	4.3	1.93	-4.312	10.49	153	5	107.87
14	Fe	3.13	-1.16	-1.16	3.14	-4.3	26	8	132	3.844	2.5	4.31	1.83	167.82	7.874	125	4	55.845
15	Ce	1.81	-1.13	-1.13	3.08	-4.2	58	NA	204	3.486	NA	NA	1.12	0.1975	6.689	174	6	140.12
16	Ge	1.07	-4.19	-4.19	-0.02	-4.17	32	14	120	3.757	NA	4.6	2.01	-1.786	5.323	122	4	72.631
17	K	2.1	-0.76	-0.76	3.23	-3.98	19	1	203	4.022	0.11	2.22	0.82	-2.083	0.856	243	4	39.098
18	Sn	3.28	-3.51	-3.51	-0.01	-3.78	50	14	139	3.592	0.88	4.38	1.96	-126.32	7.31	141	5	118.711
19	Ac	3.13	-0.24	-0.24	3.13	-3.77	89	NA	215	3.922	0.62	NA	1.1	-2.9502	10.07	186	7	227.028
20	Eu	3.13	-0.23	-0.23	3.22	-3.75	63	NA	198	3.992	0.49	NA	NA	167.34	5.244	208	6	151.96
21	Ca	3.13	-0.36	-0.36	3.16	-3.66	20	2	176	3.332	0.41	2.8	1	-34.27	1.55	174	4	40.078
22	Co	3.13	-0.36	-0.36	3.16	-3.66	27	9	126	2.884	2.11	5	1.88	66.66	8.9	126	4	58.933
23	Am	3.13	-0.3	-0.3	3.18	-3.63	95	NA	180	4.069	NA	NA	1.3	-5.368	13.67	173	7	243.06
24	Er	3.13	-0.35	-0.35	3.18	-3.54	68	NA	189	3.179	NA	NA	1.24	167.04	9.066	176	6	167.259
25	Tl	1.2	-3.26	-3.26	1.64	-3.27	81	13	190	3.901	0.29	3.7	1.62	-112.51	11.85	144	6	204.383
26	Ba	0.9	-2.41	-2.41	-0.05	-2.38	56	2	215	3.475	0.31	2.49	0.89	149.42	3.51	198	6	137.328
27	Yb	1.32	-2.09	-2.09	-0.04	-2.33	70	NA	187	3.395	0.48	NA	NA	-46.095	6.57	187	6	173.055
28	Sr	3.13	-2.31	-2.31	-0.05	-2.26	38	2	195	3.343	0.35	2.35	0.95	-36.01	2.63	192	5	87.62
29	Zn	3.13	-2.05	-2.05	-0.01	-2.04	30	12	122	3.317	0.32	4.24	1.65	-22.34	7.14	131	4	65.38
30	Pt	2.59	-1.88	-1.88	-0.17	-1.72	78	10	136	3.065	1.85	5.6	2.28	-3.6964	21.45	128	6	195.08
31	Mg	3.13	-3.39	-3.39	0	-1.53	12	2	141	3.085	0.55	3.64	1.31	-18.43	1.738	150	3	24.305
32	Ru	0.93	-1.39	-1.39	0	-1.38	44	8	220	3.213	2.52	4.7	2.2	-7.7162	12.37	130	5	101.08
33	Ta	0.89	-1.36	-1.36	-0.08	-1.28	73	5	170	3.176	2.47	4.5	1.5	-4.7924	16.65	138	6	180.948
34	Zr	2.28	-1.16	-1.16	0	-1.24	40	4	175	3.029	1.57	4.3	1.33	-12.068	6.511	155	4	91.224
35	Mo	3.13	-1.39	-1.39	-0.18	-1.22	42	6	154	3.085	2.73	4.4	2.16	-3.8755	10.28	139	5	95.95
36	Re	1.42	-1.16	-1.16	0	-1.2	75	7	151	3.1	2.61	4.9	1.9	-4.2923	21.02	137	6	186.207
37	W	2.1	-1.38	-1.38	-0.18	-1.2	74	6	162	3.091	4.02	4.5	2.36	-1.2161	19.25	139	6	183.85
38	Rh	2.58	-1.36	-1.36	-0.17	-1.19	45	9	142	3.005	2.35	4.9	2.28	-8.62	12.45	134	5	102.906
39	Hf	3.13	-1.06	-1.06	0	-1.19	72	4	175	1.196	1.73	4.5	1.3	155.65	13.31	155	6	178.49
40	Nb	1.15	-1.32	-1.32	-0.16	-1.17	41	5	164	3.276	2.06	3.99	1.6	-5.9784	8.57	146	5	92.906
41	Y	3.13	-1.04	-1.04	0	-1.14	39	3	190	3.252	1	3.2	1.22	-11.7035	4.472	180	5	88.906
42	Lu	3.13	-1.09	-1.09	-4.47	-1.09	71	NA	187	3.496	1.6	NA	1.27	-7.2193	9.841	174	6	174.967
43	Li	1.56	-1.4	-1.4	-0.42	-1.03	3	1	128	2.748	0.49	2.38	0.98	166.01	0.535	128	2	6.941
44	Os	1.48	-0.91	-0.91	0	-0.92	76	8	144	3.199	2.96	5.1	2.2	-6.6	22.59	130	6	190.23
45	Na	3.13	-1.07	-1.07	-0.19	-0.88	11	1	166	3.059	0.21	2.35	0.93	-3.3092	0.968	190	3	22.99
46	Tc	3.13	-0.38	-0.38	0	-0.75	43	7	147	3.182	2.21	NA	1.9	-8.3145	11.5	NA	5	98.907
47	Rb	3.13	-0.66	-0.66	-0.02	-0.72	37	1	220	3.576	0.08	2.16	0.82	-4.0301	1.532	303	5	85.468
48	Gd	1.65	-0.71	-0.71	0	-0.71	64	NA	196	3.529	NA	NA	1.2	166.26	7.901	NA	6	157.25
49	Cs	3.13	-0.64	-0.64	-0.01	-0.7	55	1	244	3.686	0.06	1.81	0.79	165.02	1.879	298	6	132.905
50	Dy	3.13	-0.69	-0.69	0	-0.69	66	NA	192	3.144	NA	NA	1.22	166.63	8.551	NA	6	162.5
51	Cr	2.08	-0.78	-0.78	-0.19	-0.65	24	6	139	3.143	3.06	4.5	1.66	166.1	7.19	127	4	51.996
52	Sc	3.13	-0.56	-0.56	0	-0.62	21	3	170	3.241	1.26	3.5	1.36	-3.2482	2.985	170	4	44.956
53	V	3.13	-0.56	-0.56	-0.09	-0.59	23	5	153	3.074	2.4	4.1	1.63	-1.0147	6.11	134	4	50.942
54	Th	3.13	-0.25	-0.25	-0.04	-0.59	90	NA	206	3.292	1.15	NA	1.3	-4.1622	11.724	NA	7	232.038
55	La	3.13	-0.57	-0.57	0	-0.58	57	NA	207	3.253	0.71	NA	1.1	163.84	6.146	NA	6	138.905
56	Ti	2.79	-0.27	-0.27	0	-0.46	22	4	160	3.559	1.97	4.3	1.54	-3.1252	4.507	176	4	47.88
57	Nd	3.13	-0.15	-0.15	-7.16	-0.29	60	NA	201	3.444	NA	NA	1.14	-2	7.01	NA	6	144.243
58	Tb	3.13	-0.14	-0.14	0	-0.28	65	NA	194	3.23	NA	NA	NA	-0.1089	8.219	NA	6	158.925
59	Tm	3.13	-0.14	-0.14	0	-0.28	69	NA	190	4.314	NA	NA	1.25	-1.1247	9.32	NA	6	168.934
60	Ho	2.03	-0.05	-0.05	0	-0.15	67	NA	192	5.471	NA	NA	1.23	166.67	8.795	NA	6	164.93
61	Pr	3.13	-0.19	-0.19	-5.74	0.34	59	NA	203	3.422	NA	NA	1.13	3.8232	6.64	NA	6	140.908