

Understanding the binding interaction of imidazole with ZnO nanomaterials and clusters

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Table S1. Mulliken atomic charges of imidazole and imidazole–Zn_nO_n clusters (n = 1-4)

S. No.	Imidazole		Imidazole-Zn ₂ O ₂		Imidazole-Zn ₃ O ₃		Imidazole-Zn ₄ O ₄ (R)		Imidazole-Zn ₄ O ₄ (W)	
	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges
1	C	-0.057107	C	0.007123	C	0.086970	C	0.023717	C	0.026088
2	C	-0.029555	C	-0.056496	C	-0.097122	C	-0.618156	C	-0.109449
3	C	0.048013	C	0.134347	C	0.162095	C	-0.022226	C	0.086707
4	C	-0.005005	C	0.002228	C	0.069403	C	-0.046402	C	-0.077401
5	C	-0.120660	C	-0.487496	C	-0.614764	C	-0.106073	C	-0.297884
6	C	-0.099602	C	-0.078886	C	-0.053578	C	-0.077795	C	-0.060070
7	C	-0.136034	C	-0.105115	C	-0.124518	C	-0.140304	C	-0.097378
8	H	0.135708	H	0.455771	H	0.398768	H	0.133375	H	0.343947
9	C	-0.136127	C	-0.081080	C	-0.154350	C	-0.121525	C	-0.101037
10	H	0.156103	H	0.185200	C	-0.075124	H	0.194032	H	0.177666
11	C	-0.127497	C	-0.132400	H	0.106447	C	-0.111615	C	-0.128083
12	H	0.127732	H	0.129447	H	0.126442	H	0.131678	H	0.104038
13	H	0.129724	H	0.156542	H	0.113865	H	0.145102	H	0.138479
14	H	0.127934	H	0.133485	C	0.121308	H	0.134135	H	0.130123
15	C	-0.023749	C	0.013090	C	-0.325636	C	-0.036650	C	-0.052737
16	C	-0.105187	C	-0.484446	C	-0.096333	C	-0.102543	C	-0.296394
17	C	-0.105386	C	-0.128517	C	-0.203044	C	-0.100102	C	-0.124185
18	C	-0.134155	C	-0.097901	H	0.357177	C	-0.131121	C	-0.138256
19	H	0.143437	H	0.461469	C	-0.117298	H	0.144195	H	0.348939
20	C	-0.132856	H	0.142987	H	0.155028	C	-0.131446	C	-0.099747
21	H	0.137291	C	-0.131777	C	-0.093583	H	0.137175	H	0.145792
22	C	-0.120219	H	0.134682	H	0.175262	C	-0.111864	C	-0.127837

23	H	0.134470	H	0.133298	H	0.143012	H	0.138756	H	0.115488
24	H	0.133182	N	-0.157781	H	0.138703	H	0.136341	H	0.132095
25	H	0.132255	N	-0.058742	N	-0.154744	H	0.136531	H	0.134573
26	N	-0.128682	C	-0.021020	N	-0.056986	N	-0.161838	N	-0.112989
27	N	-0.122575	C	-0.122379	C	-0.020894	N	-0.088610	N	-0.020947
28	C	0.040678	C	-0.128560	C	-0.131996	C	0.017059	C	-0.036648
29	C	-0.116009	C	-0.059539	C	-0.124189	C	-0.117189	C	-0.124894
30	C	-0.125579	H	0.157376	C	-0.062526	C	-0.115530	C	-0.122196
31	C	-0.060595	C	-0.073517	H	0.153036	C	-0.053317	C	-0.067526
32	H	0.149195	H	0.151367	C	-0.072560	H	0.155751	H	0.155451
33	C	-0.063025	C	-0.113112	H	0.153985	C	-0.060760	C	-0.079860
34	H	0.148502	H	0.142252	C	-0.114722	H	0.150113	H	0.153359
35	C	-0.122292	C	-0.166251	H	0.142080	C	-0.116675	C	-0.118168
36	H	0.134839	H	0.092987	C	-0.166498	H	0.139821	H	0.137202
37	C	-0.172273	H	0.087517	H	0.092123	C	-0.174123	C	-0.165031
38	H	0.087977	H	0.082079	H	0.087624	H	0.091470	H	0.089150
39	H	0.085099	C	-0.166804	H	0.084499	H	0.087936	H	0.083300
40	H	0.085725	H	0.091622	C	-0.167117	H	0.086898	H	0.082718
41	C	-0.172439	H	0.091067	H	0.087629	C	-0.175399	C	-0.164851
42	H	0.089635	H	0.086032	H	0.090620	H	0.092406	H	0.088324
43	H	0.087851	C	-0.048626	H	0.087727	H	0.092255	H	0.087663
44	H	0.082039	C	-0.120181	C	-0.058787	H	0.087500	H	0.081853
45	C	0.019898	O	-0.068699	C	-0.116327	C	-0.012722	C	-0.050848
46	C	-0.174364	C	-0.211402	O	-0.041232	C	-0.107090	C	-0.142668
47	O	-0.069300	H	0.193899	C	-0.219953	O	-0.079810	O	-0.053385
48	C	-0.202711	C	-0.025279	H	0.186393	C	-0.196283	C	-0.222024
49	H	0.165015	H	0.168353	C	-0.008718	H	0.174637	H	0.187906

50	C	-0.079301	H	0.198518	H	0.165033	C	-0.036437	C	-0.012067
51	H	0.159898	Zn	0.491535	H	0.201547	H	0.172689	H	0.159068
52			Zn	0.452374	H	0.121149	H	0.208729	H	0.199529
53			O	-0.651078	Zn	0.573345	Zn	0.604153	Zn	0.654963
54			O	-0.626696	Zn	0.527833	Zn	0.581373	Zn	0.397150
55					Zn	0.526537	Zn	0.569357	Zn	0.555686
56					O	-0.672536	Zn	0.579639	Zn	0.569624
57					O	-0.672348	O	-0.728685	O	-0.618268
58					O	-0.618156	O	-0.721883	O	-0.488531
59							O	-0.637002	O	-0.643044
60							O	-0.649077	O	-0.612475

Table S2. Mulliken atomic charges of imidazole–Zn_nO_n clusters (n = 5-9)

S. No.	Imidazole-Zn ₅ O ₅		Imidazole-Zn ₆ O ₆ (R)		Imidazole-Zn ₆ O ₆ (C)		Imidazole-Zn ₇ O ₇		Imidazole-Zn ₈ O ₈		Imidazole-Zn ₉ O ₉	
	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges	Atoms	Atomic charges
1	C	0.215899	C	0.202298	C	0.197438	C	0.214651	C	0.154743	C	0.159144
2	C	0.265311	C	0.260134	C	0.216178	C	0.262689	C	0.274270	C	0.322534
3	C	0.502270	C	0.484396	C	0.508376	C	0.490263	C	0.410593	C	0.474476
4	C	0.155269	C	0.211224	C	0.275701	C	0.219269	C	0.251748	C	0.243441
5	C	-0.295349	C	-0.298039	C	-0.508954	C	-0.301495	C	-0.283859	C	-0.284677
6	C	-0.034249	C	-0.031317	C	-0.184342	C	-0.042826	C	-0.412372	C	-0.233464
7	C	-0.272960	C	-0.267472	C	-0.242810	C	-0.267382	C	-0.307915	C	-0.281969
8	H	0.220692	H	0.236455	H	0.431581	H	0.239399	H	0.221097	H	0.250712
9	C	-0.245651	C	-0.213675	C	-0.268388	C	-0.216757	C	-0.193617	C	-0.219932
10	H	0.230020	H	0.101740	H	0.132969	H	0.099939	H	0.411072	H	0.507525
11	C	-0.260955	C	-0.267762	C	-0.226495	C	-0.274572	C	-0.262474	C	-0.254411
12	H	0.208455	H	0.215449	H	0.209864	H	0.216894	H	0.207959	H	0.231851
13	H	0.113166	H	0.148040	H	0.229936	H	0.160011	H	0.203141	H	0.171895
14	H	0.211462	H	0.217141	H	0.219709	H	0.219660	H	0.214690	H	0.230768
15	C	0.166322	C	0.200233	C	0.221941	C	0.204836	C	0.212051	C	0.191882
16	C	-0.371447	C	-0.377842	C	-0.497089	C	-0.384872	C	-0.367561	C	-0.345943
17	C	-0.249368	C	-0.258674	C	-0.264039	C	-0.257423	C	-0.269859	C	-0.265025
18	C	-0.209118	C	-0.228449	C	-0.236336	C	-0.228566	C	-0.233717	C	-0.245319
19	H	0.246788	H	0.260089	H	0.425145	H	0.264449	H	0.261452	H	0.253325
20	C	-0.246946	C	-0.244617	C	-0.262263	C	-0.248670	C	-0.250155	C	-0.253660
21	H	0.223615	H	0.230544	H	0.251833	H	0.230419	H	0.228686	H	0.237285
22	C	-0.222834	C	-0.221009	C	-0.223245	C	-0.219418	C	-0.220987	C	-0.220792

23	H	0.214037	H	0.220539	H	0.211777	H	0.219879	H	0.215180	H	0.226756
24	H	0.213747	H	0.215179	H	0.219085	H	0.215675	H	0.213895	H	0.222188
25	H	0.218835	H	0.220593	H	0.218516	H	0.220623	H	0.214923	H	0.226175
26	N	-0.731041	N	-0.740330	N	-0.767574	N	-0.745901	N	-0.688924	N	-0.741024
27	N	-0.611511	N	-0.592969	N	-0.535823	N	-0.590665	N	-0.541073	N	-0.555084
28	C	0.313133	C	0.307673	C	0.311856	C	0.305113	C	0.323775	C	0.324514
29	C	-0.372330	C	-0.378471	C	-0.355091	C	-0.374010	C	-0.354570	C	-0.360195
30	C	-0.447409	C	-0.466652	C	-0.610265	C	-0.470596	C	-0.493646	C	-0.493761
31	C	0.317964	C	0.309525	C	0.303092	C	0.306068	C	0.323737	C	0.318518
32	H	0.238490	H	0.246340	H	0.277809	H	0.247209	H	0.239290	H	0.242436
33	C	0.336295	C	0.346107	C	0.369940	C	0.343766	C	0.356716	C	0.359412
34	H	0.261091	H	0.269123	H	0.319581	H	0.267629	H	0.257945	H	0.261135
35	C	-0.470147	C	-0.469092	C	-0.472770	C	-0.466943	C	-0.479925	C	-0.468408
36	H	0.229068	H	0.231721	H	0.233552	H	0.232478	H	0.229673	H	0.230580
37	C	-0.628043	C	-0.625556	C	-0.637946	C	-0.625292	C	-0.642744	C	-0.631805
38	H	0.199666	H	0.201307	H	0.210003	H	0.201676	H	0.199123	H	0.198510
39	H	0.185296	H	0.185428	H	0.188156	H	0.185018	H	0.183187	H	0.185775
40	H	0.187342	H	0.186653	H	0.180641	H	0.186939	H	0.180698	H	0.181651
41	C	-0.632951	C	-0.630142	C	-0.630103	C	-0.630465	C	-0.639124	C	-0.633548
42	H	0.204515	H	0.206051	H	0.203409	H	0.206297	H	0.201826	H	0.202540
43	H	0.189713	H	0.190390	H	0.196724	H	0.191485	H	0.192762	H	0.194045
44	H	0.185389	H	0.186298	H	0.187441	H	0.186240	H	0.182006	H	0.185129
45	C	0.282959	C	0.297116	C	0.229517	C	0.291684	C	0.355055	C	0.248057
46	C	-0.222427	C	-0.202391	C	-0.045733	C	-0.191737	C	-0.203574	C	-0.176400
47	O	-0.466524	O	-0.504479	O	-0.535881	O	-0.517761	O	-0.530497	O	-0.520222
48	C	-0.316891	C	-0.293339	C	-0.324549	C	-0.293713	C	-0.275428	C	-0.286529
49	H	0.272528	H	0.271532	H	0.212054	H	0.272619	H	0.271414	H	0.280646

50	C	0.054107	C	0.027085	C	0.032698	C	0.030346	C	-0.027046	C	0.046740
51	H	0.245117	H	0.249454	H	0.247757	H	0.248718	H	0.241574	H	0.255332
52	H	0.264645	H	0.260371	H	0.260829	H	0.257644	H	0.263303	H	0.265945
53	Zn	1.274016	Zn	1.232666	Zn	1.273945	Zn	1.236659	Zn	0.998877	Zn	1.153242
54	Zn	1.046884	Zn	0.968407	O	-1.080970	Zn	1.009533	Zn	1.079898	Zn	0.526775
55	Zn	1.023506	Zn	1.020784	O	-1.274665	Zn	1.002989	Zn	1.087440	Zn	0.825913
56	Zn	1.027888	Zn	1.022683	O	-1.048246	Zn	1.024237	Zn	1.097221	Zn	0.989933
57	Zn	0.998959	O	-1.072871	Zn	1.192262	O	-1.083846	Zn	1.109634	Zn	1.054232
58	O	-1.149090	O	-1.062368	Zn	0.898472	O	-1.065071	Zn	1.081871	Zn	1.138587
59	O	-1.062006	O	-1.097030	Zn	1.189188	O	-1.087889	Zn	1.030178	Zn	1.140991
60	O	-1.035414	O	-1.092610	Zn	0.904094	O	-1.095215	Zn	1.289733	Zn	1.042693
61	O	-1.092543	O	-1.043988	Zn	1.104771	O	-0.990064	O	-1.017328	Zn	1.001881
62	O	-1.097255	O	-1.049046	O	-1.236096	Zn	0.984519	O	-1.158005	O	-0.551415
63			Zn	1.024570	O	-1.032469	Zn	1.038209	O	-1.096299	O	-1.119396
64			Zn	1.064849	O	-0.995699	Zn	1.036524	O	-1.102580	O	-1.078114
65							O	-1.044973	O	-1.109153	O	-1.065553
66							O	-1.056134	O	-1.106610	O	-1.083212
67									O	-1.091267	O	-1.152179
68									O	-1.112124	O	-1.108029
69											O	-1.103000
70											O	-1.072102