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Thermodynamic feasible photoelectron transfer from bioactive π-expanded imidazole luminophore to ZnO nanocrystals

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Table S1. Mulliken atomic charges of imidazole, imidazole– Zn_nO_n clusters (n = 1-5)

S. No.	**Imidazole**		**Imidazole-ZnO**		**Imidazole-Zn_2O_2**		**Imidazole-Zn_3O_3**		**Imidazole-Zn_4O_4**		**Imidazole-Zn_5O_5**	
	Atoms	**Atomic charges**	**Atoms**	**Atomic charges**	**Atoms**	**Atomic charges**	**Atoms**	**Atomic charges**	**Atoms**	**Atomic charges**	**Atoms**	**Atomic charges**
1	C	0.015369	C	0.219342	C	0.218375	C	0.015615	C	0.041513	C	0.281339
2	C	0.160691	C	0.194925	C	0.164047	C	0.210518	C	0.223136	C	0.249987
3	C	0.148338	C	0.352964	C	0.342110	C	0.298912	C	0.194303	C	0.114692
4	C	0.148338	C	0.263731	C	0.173020	C	0.042713	C	0.119776	C	0.040415
5	C	0.243078	C	-0.227947	C	-0.193496	C	-0.105924	C	-0.101662	C	-0.090457
6	C	-0.370375	C	-0.331741	C	-0.230110	C	-0.115383	C	-0.114916	C	-0.557520
7	C	-0.151396	C	-0.156119	C	-0.186989	C	-0.239475	C	-0.251408	C	-0.156720
8	H	0.181195	H	0.203519	H	0.168389	H	0.249381	H	0.266894	H	0.204256
9	C	-0.283833	C	-0.281675	C	-0.326713	C	-0.260508	C	-0.404901	C	-0.122240
10	H	0.242337	H	0.343732	H	0.297410	H	0.238118	H	0.205496	H	0.544739
11	C	-0.309906	C	-0.305388	C	-0.314652	C	-0.336590	C	-0.293556	C	-0.348353
12	H	0.187431	H	0.190186	H	0.184032	H	0.202279	H	0.202521	H	0.223179
13	H	0.207261	H	0.222317	H	0.219417	H	0.214179	H	0.230151	H	0.213374
14	H	0.226049	H	0.230071	H	0.220959	H	0.221650	H	0.223184	H	0.238906
15	C	0.350506	C	0.335721	C	0.360376	C	0.307055	C	0.255215	C	0.277795
16	C	-0.334154	C	-0.329816	C	-0.347918	C	-0.329784	C	-0.319504	C	-0.301100
17	C	-0.350853	C	-0.279005	C	-0.328620	C	-0.207801	C	-0.116250	C	-0.074045
18	C	-0.322119	C	-0.326517	C	-0.328519	C	-0.327880	C	-0.321886	C	-0.329283
19	H	0.245120	H	0.236599	H	0.232256	H	0.234999	H	0.232420	H	0.265331
20	C	-0.140124	C	-0.134994	C	-0.140305	C	-0.187925	C	-0.209799	C	-0.223754
21	H	0.323001	H	0.208857	H	0.272420	H	0.296889	H	0.211664	H	0.144210
22	C	-0.290052	C	-0.283172	C	-0.288212	C	-0.266152	C	-0.254047	C	0.144210

23	H	0.200868	H	0.204493	H	0.199395	H	0.204134	H	0.201466	H	0.213161
24	H	0.176283	H	0.188149	H	0.193908	H	0.194137	H	0.191955	H	0.177880
25	H	0.226571	H	0.229038	H	0.224531	H	0.220258	H	0.218924	H	0.214539
26	N	-0.196058	N	-0.568141	N	-0.630555	N	-0.483122	N	-0.555991	N	-0.673708
27	N	-0.537013	N	-0.567442	N	-0.548226	N	-0.609831	N	-0.531509	N	-0.715327
28	C	0.188581	C	0.155866	C	0.174656	C	0.147271	C	0.158939	C	0.162459
29	C	-0.167173	C	-0.159131	C	-0.165720	C	-0.149889	C	-0.160119	C	-0.242490
30	C	0.277229	C	0.381344	C	0.393959	C	0.373277	C	0.374607	C	0.326384
31	C	-0.300566	C	-0.302614	C	-0.309320	C	-0.298512	C	-0.291289	C	-0.255984
32	H	0.220821	H	0.226606	H	0.218489	H	0.227898	H	0.232136	H	0.242185
33	C	-0.387900	C	-0.385414	C	-0.391365	C	-0.391259	C	-0.380947	C	-0.346036
34	C	-0.183615	C	-0.169694	C	-0.172009	C	-0.172326	C	-0.166965	C	-0.232278
35	H	0.216708	H	0.227149	H	0.222891	H	0.225809	H	0.230569	H	0.213576
36	H	0.214973	H	0.227026	H	0.220498	H	0.222199	H	0.226219	H	0.208535
37	C	0.214854	C	0.216053	C	0.220728	C	0.249414	C	0.238819	C	0.199152
38	C	0.086853	C	0.087190	C	0.090147	C	0.083528	C	0.062283	C	0.027583
39	C	-0.214560	C	-0.216448	C	-0.205571	C	-0.226170	C	-0.232466	C	-0.239252
40	C	-0.333835	C	-0.338571	C	-0.335887	C	-0.339937	C	-0.330042	C	-0.314905
41	C	0.370329	C	0.368964	C	0.370457	C	0.372321	C	0.374587	C	0.373623
42	C	-0.253789	C	-0.262895	C	-0.262778	C	-0.262519	C	-0.257310	C	-0.249849
43	H	0.251792	H	0.243884	H	0.244552	H	0.245449	H	0.247889	H	0.282246
44	C	-0.232219	C	-0.227567	C	-0.229141	C	-0.229946	C	-0.231555	C	-0.252243
45	H	0.273189	H	0.269136	H	0.266769	H	0.270593	H	0.278624	H	0.294484
46	C	-0.391162	C	-0.387261	C	-0.388746	C	-0.391744	C	-0.392481	C	-0.406303
47	C	-0.419919	C	-0.414560	C	-0.416887	C	-0.425671	C	-0.429189	C	-0.463895
48	H	0.218326	H	0.225422	H	0.222377	H	0.220577	H	0.220767	H	0.201849
49	C	-0.233435	C	-0.231896	C	-0.232853	C	-0.232883	C	-0.232270	C	-0.234692

50	H	0.219075	H	0.224559	H	0.222612	H	0.222757	H	0.222955	H	0.209677
51	H	0.221449	H	0.225976	H	0.224098	H	0.223587	H	0.222981	H	0.213104
52	H	0.226987	H	0.233385	H	0.230895	H	0.229496	H	0.229169	H	0.215293
53	H	0.218198	H	0.223985	H	0.221721	H	0.220697	H	0.220331	H	0.206394
54	H	0.213087	H	0.231534	H	0.224967	H	0.215924	H	0.220980	H	0.200226
55	O	-0.595132	O	-0.697950	O	-0.683816	O	-0.670068	O	-0.677471	O	-0.736095
56	H	0.396445	H	0.469632	H	0.477084	H	0.415270	H	0.417559	H	0.415394
57			Zn	0.837731	Zn	1.183748	Zn	1.222681	Zn	1.242076	Zn	1.342287
58			O	-1.113128	Zn	0.925407	Zn	0.921911	O	-1.053102	Zn	1.127580
59					O	-1.050740	Zn	0.980595	O	-1.090686	Zn	0.833465
60					O	-1.117551	O	-1.061861	O	-0.971709	O	-0.884671
61							O	-0.988969	O	-1.066436	O	-1.036128
62							O	-1.129960	Zn	0.927935	O	-0.969446
63									Zn	1.092103	Zn	1.002395
64									Zn	0.979322	O	-1.087133
65											Zn	1.068486
66											O	-0.977631

Table S2. Mulliken atomic charges of imidazole–Zn_nO_n clusters (n = 6-9)

S. No.	Imidazole-Zn_6O_6		Imidazole-Zn_7O_7		Imidazole-Zn_8O_8		Imidazole-Zn_9O_9	
	Atoms	**Atomic charges**	**Atoms**	**Atomic charges**	**Atoms**	**Atomic charges**	**Atoms**	**Atomic charges**
1	C	0.081996	C	0.030282	C	0.030282	C	0.246294
2	C	0.127220	C	0.030282	C	0.159546	C	0.138339
3	C	0.389323	C	0.411610	C	0.411610	C	0.526128
4	C	0.380612	C	0.342494	C	0.342494	C	0.349627
5	C	-0.374945	C	-0.188895	C	-0.188895	C	-0.184606
6	C	-0.281298	C	-0.279035	C	-0.279035	C	-0.379258
7	C	-0.162007	C	-0.233997	C	-0.233997	C	-0.183644
8	H	0.186415	H	0.110917	H	0.110917	H	0.061182
9	C	0.041152	C	-0.169194	C	-0.169194	C	-0.258516
10	H	0.062879	H	0.117255	H	0.117255	H	0.209977
11	C	-0.347672	C	-0.299123	C	-0.299123	C	-0.256841
12	H	0.203029	H	0.213948	H	0.213948	H	0.204469
13	H	0.205310	H	0.217749	H	0.217749	H	0.214406
14	H	0.239598	H	0.247196	H	0.247196	H	0.249173
15	C	0.365285	C	0.210541	C	0.210541	C	0.373193
16	C	-0.336136	C	-0.318020	C	-0.318020	C	-0.339953
17	C	-0.309994	C	-0.188449	C	-0.188449	C	-0.301399
18	C	-0.303072	C	-0.234457	C	-0.234457	C	-0.318317
19	H	0.229096	H	0.229902	H	0.229902	H	0.239257
20	C	-0.151374	C	-0.180776	C	-0.180776	C	-0.152313
21	H	0.314287	H	0.236882	H	0.236882	H	0.291239
22	C	-0.252866	C	-0.253144	C	-0.253144	C	-0.269793

23	H	0.196485	H	0.219011	H	0.219011	H	0.202874
24	H	0.190277	H	0.209504	H	0.209504	H	0.186953
25	H	0.219706	H	0.233508	H	0.233508	H	0.226935
26	N	-0.671809	N	-0.497215	N	-0.497215	N	-0.804517
27	N	-0.549308	N	-0.603205	N	-0.603205	N	-0.603467
28	C	0.140475	C	0.028466	C	0.028466	C	0.191302
29	C	-0.130066	C	0.001343	C	0.001343	C	-0.128572
30	C	0.430183	C	0.375921	C	0.375921	C	0.349579
31	C	-0.306147	C	-0.309529	C	-0.309529	C	-0.308053
32	H	0.228846	H	0.180865	H	0.180865	H	0.215838
33	C	-0.366567	C	-0.391023	C	-0.391023	C	-0.386090
34	C	-0.172113	C	-0.127433	C	-0.127433	C	-0.161597
35	H	0.227379	H	0.230457	H	0.230457	H	0.224285
36	H	0.226399	H	0.222888	H	0.222888	H	0.221144
37	C	0.173563	C	-0.069290	C	-0.069290	C	0.226004
38	C	0.111559	C	0.184214	C	0.184214	C	0.085631
39	C	-0.195023	C	-0.153519	C	-0.153519	C	-0.223171
40	C	-0.346394	C	-0.351590	C	-0.351590	C	-0.326303
41	C	0.367598	C	0.304790	C	0.304790	C	0.381639
42	C	-0.255344	C	-0.249828	C	-0.249828	C	-0.263286
43	H	0.246866	H	0.232839	H	0.232839	H	0.243592
44	C	-0.220065	C	-0.215280	C	-0.215280	C	-0.228378
45	H	0.262628	H	0.246816	H	0.246816	H	0.271859
46	C	-0.380085	C	-0.334883	C	-0.334883	C	-0.388519
47	C	-0.406290	C	-0.349915	C	-0.349915	C	-0.421106
48	H	0.220754	H	0.214909	H	0.214909	H	0.220507
49	C	-0.228162	C	-0.225051	C	-0.225051	C	-0.228368

50	0.220189	H	0.212880	H	0.212880	H	0.224677
51	0.223860	H	0.217473	H	0.217473	H	0.222992
52	0.230576	H	0.225619	H	0.225619	H	0.231264
53	0.221784	H	0.220805	H	0.220805	H	0.221965
54	0.256733	H	0.223205	H	0.223205	H	0.215740
55	-0.833827	O	-0.607110	O	-0.607110	O	-0.631834
56	0.521618	H	0.408540	H	0.408540	H	0.408571
57	0.977659	Zn	0.905208	Zn	0.905208	Zn	1.096638
58	1.063634	Zn	1.070956	Zn	1.070956	Zn	1.083851
59	1.081525	Zn	1.055045	Zn	1.055045	Zn	1.088251
60	1.051181	Zn	1.054664	Zn	1.054664	Zn	1.063189
61	1.142146	Zn	1.037489	Zn	1.037489	Zn	1.129516
62	1.297015	Zn	1.038231	Zn	1.038231	Zn	1.087209
63	-1.118431	Zn	0.981266	Zn	0.981266	Zn	1.046960
64	-1.099285	Zn	1.172236	Zn	1.172236	Zn	1.070058
65	-1.079629	O	-0.974166	O	-0.974166	Zn	1.257823
66	-1.124653	O	-1.070314	O	-1.070314	O	-1.219505
67	-1.225663	O	-1.109742	O	-1.109742	O	-1.103437
68	-1.128616	O	-1.066156	O	-1.066156	O	-1.112812
69		O	-1.046372	O	-1.046372	O	-1.058769
70		O	-1.074907	O	-1.074907	O	-1.108688
71		O	-1.057891	O	-1.057891	O	-1.133787
72		O	-1.007957	O	-1.007957	O	-1.069287
73						O	-1.057571
74						O	-1.188372