Supplementary Material for PCCP

ELECTRIC SUPPLEMENTARY INFORMATION (ESI)

The Structures and Electronic States of Zinc-Water Clusters $Zn_n(H_2O)_m$ (n=1-32 and m=1-3)

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Cartesian coordinates of large clusters are given below.

n=20

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	4.936169	-0.285854	-0.840115
2	30	0	0.713867	3.422807	-1.233551
3	30	0	2.356038	-2.087050	-1.923491
4	30	0	-0.366605	1.064246	-2.634872
5	30	0	-2.145924	2.998993	-1.316813
6	30	0	-0.616944	-1.962028	-2.631451
7	30	0	-2.858424	-0.089936	-1.802029
8	30	0	2.624848	-1.083237	0.782913
9	30	0	2.369205	0.897925	-1.508827
10	30	0	-0.884806	3.568945	1.268007
11	30	0	0.137383	-2.868392	0.054764
12	30	0	-2.630592	1.146923	0.810551
13	30	0	-2.766423	-2.888755	-0.817823
14	30	0	2.173311	0.228633	3.384647
15	30	0	1.594838	1.897200	1.068868
16	30	0	0.637221	-2.227253	2.859334
17	30	0	-0.165561	-0.059033	-0.069049
18	30	0	-0.608211	0.948882	2.699411
19	30	0	-2.043874	-1.621456	1.717735
20	30	0	-4.891776	-0.902111	0.426856
21	8	0	7.196963	-0.296464	-0.884601
22	1	0	7.769436	0.324209	-0.368969

23	1	0	7.742658	-0.935998	-1.406202

n=24

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.167452	3.556803	-1.143507
2	30	0	2.896158	1.953443	-1.571050
3	30	0	-1.706500	2.469010	0.799679
4	30	0	1.092438	1.518102	0.716639
5	30	0	4.468089	-0.511365	-1.169571
6	30	0	-0.434586	2.068628	3.335867
7	30	0	2.039870	0.373011	3.193564
8	30	0	-2.236033	2.172198	-2.116986
9	30	0	1.275066	-0.394957	-1.492865
10	30	0	2.604471	-2.821360	-0.837218
11	30	0	-1.153928	-0.103764	-0.102250
12	30	0	0.950445	-1.489208	1.243571
13	30	0	-0.720879	-0.803230	3.684747
14	30	0	-1.243115	-0.436436	-2.898355
15	30	0	0.266987	-2.964780	-2.792913
16	30	0	-4.447024	1.480372	-0.354664
17	30	0	-2.551141	-2.569688	-1.428348
18	30	0	-0.181722	-3.925059	-0.126794
19	30	0	-4.607538	-1.382917	0.201704
20	30	0	-1.935744	-2.248627	1.505248
21	30	0	0.496685	1.849433	-3.397148
22	30	0	-3.307405	0.377182	2.219036
23	30	0	3.917929	-1.540434	1.613852
24	30	0	4.111833	1.453643	1.170412
25	8	0	0.678529	5.658113	-0.780320
26	1	0	0.918410	5.972888	0.124066
27	1	0	0.799185	6.362242	-1.461001

n=28

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.070660	-2.488996	2.557250
2	30	0	-3.850143	-1.980681	0.831897
3	30	0	3.188665	-0.206241	2.327488
4	30	0	0.198004	0.193512	2.449631
5	30	0	-2.819173	0.721478	2.316715
6	30	0	-0.649300	2.924178	2.654753
7	30	0	-2.948545	3.246036	0.891711
8	30	0	2.322766	-3.532242	-2.097899
9	30	0	0.700692	-1.446997	-0.140600
10	30	0	-1.916983	-2.424712	-1.449426
11	30	0	0.798665	1.417886	-0.148667

12	30	0	-1.620526	0.085388	-0.082136
13	30	0	-0.160576	4.179780	0.145772
14	30	0	2.516993	-0.379329	-2.110379
15	30	0	0.207986	-1.648818	-3.191417
16	30	0	4.532728	0.349131	-0.185886
17	30	0	0.384655	1.286031	-3.061914
18	30	0	-2.246135	0.042822	-3.174231
19	30	0	3.049189	2.514320	-1.987121
20	30	0	-1.789579	2.504333	-1.626227
21	30	0	-0.931885	-3.764588	0.840267
22	30	0	3.041045	2.621456	1.340978
23	30	0	-4.630026	1.218889	-0.204821
24	30	0	-1.825134	-1.921457	2.901539
25	30	0	-4.584408	-1.142358	-1.912278
26	30	0	1.759226	-4.867326	0.448876
27	30	0	2.551893	4.924254	-0.492871
28	30	0	3.555418	-2.553716	0.550981
29	1	0	1.068921	0.537135	5.295581
30	8	0	0.289315	0.350395	4.719337
31	1	0	-0.568544	0.498733	5.190240

n=32

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	1.164053	3.327729	-0.467185
2	30	0	2.451509	0.440182	3.306405
3	30	0	-1.739716	3.263912	-1.620368
4	30	0	-0.810237	1.611335	0.711463
5	30	0	-0.475860	1.022474	3.487717
6	30	0	-3.212746	1.199247	2.396544
7	30	0	-2.095402	-1.356300	3.271646
8	30	0	4.864703	0.301394	-1.387038
9	30	0	1.397254	0.403777	-0.738520
10	30	0	3.342604	-0.971781	0.869377
11	30	0	-1.296888	-0.776510	-0.699515
12	30	0	0.419405	-0.886640	1.589894
13	30	0	-3.643438	-1.383879	0.796842
14	30	0	0.342789	-0.836937	-2.995359
15	30	0	2.732698	-2.159319	-1.887203
16	30	0	-2.173533	0.699498	-3.098628
17	30	0	-0.026520	-3.352896	-1.646643
18	30	0	1.678769	-3.455135	0.693605
19	30	0	-2.233753	-2.320019	-3.401282
20	30	0	-1.341164	-3.095247	1.049511
21	30	0	3.370579	1.897569	0.695700
22	30	0	-3.561828	1.173524	-0.542589
23	30	0	0.270321	-2.857284	4.018655
24	30	0	1.337960	3.004099	2.435901
25	30	0	3.163493	-2.566604	3.293225
26	30	0	3.530025	2.847362	-2.210512
27	30	0	-4.581274	-1.138624	-2.083784

28	30	0	0.524627	2.078341	-3.088392
29	30	0	-3.701441	3.762688	0.849058
30	30	0	-0.977875	4.564970	1.727517
31	30	0	2.976304	0.414985	-3.598150
32	30	0	-3.255154	-3.697764	-1.149911
33	1	0	4.991971	-3.409302	-0.839551
34	8	0	4.593966	-3.410885	-1.766100
35	1	0	5.048394	-4.047997	-2.371011
