Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Benchmark Calculations of Excess Electron in Water Cluster Cavity: Balancing the Additions of Atom-Centered Diffuse Functions versus Floating Diffuse Functions

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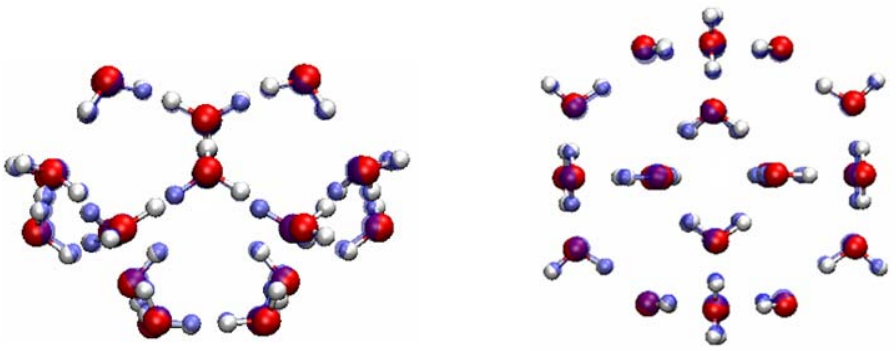
Supporting Information

Contents

1. Structures of Water Cluster Anions



$5^{12}6^2$ B **4^66^8 B**

Figure S1. The optimized structures for two isomers, $5^{12}6^2$B and 4^66^8B, of water cluster anions at different levels. The solid structures are optimized at the X3LYP/6-31++G(d) level and the blue ones are optimized at the B3LYP/6-311+3+G(d) level. The corresponding coordinates in angstrom are given in Table S1.

Table S1. The structure coordinates for $5^{12}6^{2}$B and $4^{6}6^{8}$B. The unit is in Å.

Isomer: n=24 ($5^{12}6^{2}$ B) Geometry: X3LYP/6-31++G(d)

	X	Y	Z		X	Y	Z
O	0.000000	0.000000	0.000000	H	1.834403	0.259674	-0.672276
O	0.000000	0.000000	2.810796	H	5.916372	2.821931	3.192246
O	2.543711	0.000000	3.652892	H	3.328045	4.456343	0.038776
O	3.093090	1.956783	5.725570	H	3.666336	5.915144	4.453780
O	5.365906	3.425705	4.962496	H	-0.461757	-0.736384	3.262227
O	4.644886	5.987785	4.649991	H	-1.158989	3.027164	-0.089794
O	5.605352	7.184852	2.186276	H	-0.371641	3.256001	-2.057961
O	3.428787	8.418247	0.902837	H	0.225534	5.537593	-2.244369
O	3.036749	7.198409	-1.450522	H	2.083067	7.022660	-1.653578
O	0.268081	6.499188	-1.966499	H	3.257172	7.980277	-0.003119
O	0.174119	3.795647	-2.731011	H	4.836174	7.631443	1.725229
O	-1.256238	2.454623	-0.904762	H	5.031244	6.413461	3.843096
O	2.789218	0.397388	-0.882528	H	5.126242	4.410562	4.841796
O	3.669315	1.408383	1.516536	H	3.905427	2.481554	5.464089
O	6.186991	2.544141	2.282955	H	2.712439	0.619969	4.407039
O	6.328136	4.799057	0.604054	H	0.957472	-0.007186	3.164662
O	3.929434	4.649451	-0.729426	H	-0.372984	-0.860834	-0.280575
O	2.884490	2.677997	-2.529268	H	1.821134	8.057549	1.946040
O	0.995534	7.855399	2.450741	H	1.485225	3.089001	5.597577
O	2.004770	5.558725	3.837544	H	0.361792	3.960562	1.318048
O	0.759547	3.749815	5.490211	H	3.029180	0.405961	2.877710
O	-1.098410	2.561930	3.740362	H	6.321694	7.851364	2.225424
O	-0.630584	4.025668	1.320933	H	-0.233445	6.998999	-2.642928
O	-0.909616	6.695662	0.734489	H	-0.200258	3.589017	-3.612153
H	2.824459	1.159841	-1.529217	H	3.133803	2.245864	1.547464
H	3.448414	1.000617	0.618557	H	6.152273	5.576650	1.186497
H	5.406891	2.039145	1.931925	H	1.979349	3.066267	-2.613867
H	6.356302	4.001039	1.206695	H	2.149851	4.979879	3.041925
H	4.856851	4.657004	-0.327912	H	-0.747889	1.694496	3.421182
H	3.391540	3.338144	-1.987143	H	-0.505598	6.717294	-0.166126
H	1.248400	7.111207	3.058229	H	-0.858642	1.583945	-0.648961
H	1.485299	4.977668	4.480901	H	-0.000193	-0.011181	1.001795
H	0.058825	3.304940	4.931758	H	3.252016	1.650131	6.641881
H	-1.076897	3.151179	2.940879	H	6.138755	3.406220	5.563827
H	-0.819482	5.007562	1.173756	H	3.492633	9.380404	0.731274
H	-0.271267	7.175382	1.337161	H	3.433935	6.293228	-1.294774

Isomer: n=24 ($5^{12}6^2$ B) **Geometry: B3LYP/6-311+3+G(d)**

	X	Y	Z		X	Y	Z
O	4.129436	2.459760	-0.764238	H	3.179830	1.687393	-2.448738
O	2.358367	4.192957	0.710200	H	-3.107655	1.772535	-2.391883
O	0.047190	4.540578	-0.764889	H	-0.050386	-1.485903	-1.559526
O	-2.459276	4.128955	0.764640	H	-3.801898	0.043478	1.376686
O	-4.193045	2.358375	-0.709803	H	2.615763	5.059606	0.995590
O	-4.541329	0.047361	0.765546	H	3.801685	-0.043317	1.375771
O	-4.129597	-2.459445	-0.763518	H	4.306197	-1.534935	-0.216210
O	-2.357975	-4.192774	0.710298	H	3.010079	-3.518918	0.268514
O	-0.047087	-4.540557	-0.765226	H	0.756422	-4.455836	-0.257596
O	2.459892	-4.129169	0.763531	H	-1.534964	-4.305741	0.215594
O	4.193094	-2.357977	-0.710831	H	-3.519256	-3.009531	-0.268499
O	4.541093	-0.047110	0.764603	H	-4.456770	-0.756097	0.257808
O	2.703580	1.446522	-3.237602	H	-4.306263	1.535329	-0.215221
O	0.066556	2.103381	-2.293337	H	-3.009604	3.518971	0.269452
O	-2.665963	1.473943	-3.181353	H	-0.756192	4.455897	-0.257051
O	-2.704447	-1.446407	-3.237252	H	1.535275	4.305900	0.215627
O	-0.067246	-2.103331	-2.293551	H	4.844437	3.024372	-1.025867
O	2.665170	-1.473752	-3.181775	H	-1.772108	-3.107505	2.392256
O	-1.473378	-2.665679	3.181599	H	-1.686991	3.179453	2.449028
O	-2.103746	0.066548	2.293332	H	1.486161	-0.050176	1.558796
O	-1.446033	2.703182	3.237854	H	0.043309	3.801237	-1.376136
O	1.474253	2.665134	3.181427	H	-4.844580	-3.024193	-1.024905
O	2.103723	-0.066997	2.292708	H	3.024427	-4.844448	1.024570
O	1.446987	-2.703830	3.237327	H	5.059662	-2.615403	-0.996440
H	2.722599	0.489622	-3.280899	H	0.049704	1.485885	-1.559371
H	0.892079	1.919939	-2.749015	H	-3.180510	-1.687237	-2.448261
H	-1.745157	1.698793	-3.056187	H	3.107049	-1.772431	-2.392443
H	-2.723481	-0.489510	-3.280593	H	-1.486417	0.049674	1.559227
H	-0.892865	-1.919962	-2.749086	H	1.772695	3.107162	2.392090
H	1.744404	-1.698698	-3.056488	H	1.687870	-3.180129	2.448497
H	-1.698459	-1.744935	3.056390	H	4.456547	0.756419	0.256978
H	-1.919994	0.891952	2.749104	H	3.519320	3.009965	-0.269074
H	-0.489129	2.722234	3.281049	H	-3.023705	4.844156	1.026120
H	1.699205	1.744401	3.055886	H	-5.059618	2.616122	-0.995108
H	1.920336	-0.892504	2.748442	H	-2.615446	-5.059442	0.995562
H	0.490092	-2.722970	3.280684	H	-0.043404	-3.801219	-1.376477

Isomer: n=24 ($5^{12}6^{2}$B) **Geometry: B3LYP/6-31+G(d)-6-311+2+G(d,p++)**

	X	Y	Z
O	0.054659	0.051276	0.019058
O	0.026937	0.044890	2.782878
O	2.531696	0.082481	3.602666
O	3.079350	1.988821	5.665030
O	5.320782	3.424202	4.920125
O	4.586086	5.931860	4.569336
O	5.556370	7.121671	2.156962
O	3.417421	8.358426	0.918174
O	3.022838	7.124770	-1.376648
O	0.292907	6.466117	-1.906218
O	0.204870	3.813560	-2.677929
O	-1.156953	2.493314	-0.847800
O	2.798416	0.449588	-0.853141
O	3.636312	1.486151	1.516538
O	6.139661	2.547604	2.273838
O	6.266738	4.769024	0.607882
O	3.877765	4.608181	-0.681216
O	2.878420	2.690053	-2.496503
O	1.004370	7.817287	2.443228
O	1.994212	5.520649	3.753663
O	0.779347	3.751259	5.425965
O	-1.061536	2.574351	3.709281
O	-0.525945	4.021224	1.344096
O	-0.872347	6.655192	0.754458
H	2.824841	1.204893	-1.495841
H	3.425707	1.079266	0.625829
H	5.344766	2.079296	1.927087
H	6.295300	3.980916	1.209816
H	4.797528	4.614172	-0.284655
H	3.364636	3.336570	-1.933657
H	1.255498	7.057892	3.018899
H	1.484805	4.944187	4.395135
H	0.085343	3.306990	4.873565
H	-1.000513	3.160537	2.919467
H	-0.724818	4.991307	1.193646
H	-0.237437	7.135397	1.346449
H	1.854772	0.317472	-0.630193
H	5.883348	2.822284	3.178439
H	3.280295	4.405809	0.080502
H	3.619780	5.845773	4.351807
H	-0.411784	-0.695109	3.230055
H	-1.027733	3.056466	-0.038474
H	-0.315479	3.277261	-1.991013
H	0.252820	5.514975	-2.192647
H	2.076042	6.958393	-1.577899
H	3.239792	7.904393	0.027898
H	4.794633	7.578237	1.710192
H	4.979657	6.351417	3.773512
H	5.068076	4.396633	4.776305
H	3.891225	2.503034	5.410732
H	2.696947	0.688374	4.357530
H	0.979996	0.057950	3.131550
H	-0.311891	-0.798718	-0.268235
H	1.821749	8.022371	1.943886
H	1.508135	3.104356	5.515852
H	0.461845	3.967145	1.357309
H	2.998093	0.509023	2.835137
H	6.277346	7.768751	2.187562
H	-0.193910	6.969363	-2.576438
H	-0.192820	3.605003	-3.537217
H	3.107355	2.321537	1.539416
H	6.071742	5.538934	1.179743
H	1.981276	3.073303	-2.584481
H	2.125381	4.950001	2.956547
H	-0.719179	1.711279	3.397377
H	-0.471214	6.667227	-0.137876
H	-0.766290	1.625175	-0.607297
H	0.039807	0.036487	1.012918
H	3.218860	1.700524	6.579810
H	6.076147	3.431238	5.527904
H	3.489869	9.305961	0.725877
H	3.402259	6.221790	-1.205677
Bq	1.944314	4.109002	1.720302

Isomer: n=24 ($4^6 6^8$B) **Geometry: X3LYP/6-31++G(d)**

	X	Y	Z		X	Y	Z
O	-4.735642	0.228668	-1.320304	H	0.509247	3.208739	2.682802
O	-2.254896	0.099324	-2.512210	H	1.396640	1.337975	3.447827
O	-0.626335	-1.903906	-3.715820	H	3.220044	-0.161555	2.239705
O	-0.418905	-3.984856	-2.031394	H	4.022627	-0.957230	-1.869510
O	-2.197186	-3.759506	0.220653	H	-1.383935	4.007899	-0.560042
O	-4.268045	-1.987205	0.507184	H	-0.234708	-1.393063	3.473373
O	-4.078217	2.358259	0.563832	H	-4.579915	1.003769	-0.722621
O	-3.940922	0.150583	2.441015	H	0.155696	-1.326859	-3.500529
O	0.095029	-4.065446	1.966168	H	-1.501293	-3.796487	0.927248
O	1.892614	-3.996367	-0.293637	H	-3.224533	2.883933	0.427428
O	1.210602	-0.003995	-2.701064	H	0.264480	-3.308121	2.623567
O	-0.506782	2.028624	-3.666741	H	2.215917	-0.050077	-2.740411
O	4.735554	-0.228420	1.320257	H	4.107238	0.619077	-1.838558
O	4.267866	1.987113	-0.507472	H	-1.188729	3.914779	0.988938
O	2.197078	3.759673	-0.221280	H	1.310676	-1.515746	3.389856
O	0.419008	3.984647	2.030883	H	-4.107090	-0.619293	1.838532
O	0.626530	1.904404	3.715753	H	1.188763	-3.914952	-0.989230
O	2.255093	-0.099232	2.512848	H	-1.310613	1.515734	-3.389274
O	4.078285	-2.358316	-0.563724	H	3.224509	-2.883905	-0.427577
O	3.941069	-0.150769	-2.441083	H	-0.264742	3.308592	-2.623891
O	-0.095171	4.066058	-1.966661	H	-2.215770	0.050110	2.740739
O	-1.892595	3.996286	0.293356	H	4.579769	-1.003576	0.722664
O	-1.210433	0.004368	2.701632	H	1.501250	3.797010	-0.927925
O	0.506788	-2.028587	3.667262	H	-0.155543	1.327160	3.501133
H	-3.445104	-2.558282	0.369198	H	-1.768839	0.056959	-1.648792
H	-1.681630	-3.798783	-0.627912	H	-0.515491	-4.801086	-2.564646
H	-0.509106	-3.208817	-2.683138	H	-4.992008	-2.623531	0.681768
H	-1.396444	-1.337732	-3.447365	H	-4.763290	3.031175	0.757444
H	-3.219875	0.161671	-2.239150	H	0.091207	-4.890340	2.495179
H	-4.647790	-0.572817	-0.743476	H	1.001099	-0.012518	-1.730289
H	-4.022448	0.957015	1.869395	H	4.763365	-3.031308	-0.757064
H	1.383868	-4.007719	0.559707	H	-0.091892	4.890899	-2.495744
H	0.234755	1.393141	-3.472863	H	-1.000741	0.012579	1.730892
H	4.647393	0.572994	0.743375	H	4.991998	2.623301	-0.681847
H	3.444984	2.558320	-0.369671	H	0.515526	4.800984	2.563976
H	1.681536	3.798835	0.627308	H	1.769000	-0.057116	1.649434

Isomer: n=24 ($4^6 6^8$B) **Geometry: X3LYP/6-311+3+G(d)**

	X	Y	Z		X	Y	Z
O	-4.683827	-0.241935	-1.586842	H	0.041447	3.375888	2.743386
O	-2.081075	-0.111480	-2.775625	H	0.998173	1.527474	3.715618
O	-0.222252	-2.032568	-3.953437	H	3.011893	0.158087	2.550167
O	0.056260	-4.118502	-2.134634	H	4.345498	-0.527745	-1.731578
O	-1.839602	-4.098215	0.154244	H	-1.760178	3.900881	-0.627741
O	-4.138291	-2.461013	0.331696	H	-0.329629	-1.499543	3.798700
O	-4.380090	2.010415	0.347451	H	-4.624263	0.522535	-1.018675
O	-4.293393	-0.234924	2.303050	H	0.501459	-1.425938	-3.802369
O	0.397725	-4.115943	2.114118	H	-1.199675	-4.036962	0.860665
O	2.278365	-3.891831	-0.174709	H	-3.578323	2.540594	0.279171
O	1.522784	0.100016	-3.009953	H	0.419998	-3.370347	2.726611
O	-0.459937	2.019934	-3.940811	H	2.477779	0.147710	-2.934320
O	4.683698	0.241979	1.586814	H	4.268465	0.994112	-1.725328
O	4.138208	2.460999	-0.331804	H	-1.634370	3.891671	0.880032
O	1.839529	4.098234	-0.154514	H	1.171065	-1.427672	3.701697
O	-0.056181	4.118301	2.134468	H	-4.268303	-0.994154	1.725273
O	0.222340	2.032631	3.953637	H	1.634446	-3.891793	-0.880190
O	2.081101	0.111437	2.775907	H	-1.171073	1.427600	-3.701472
O	4.380146	-2.010434	-0.347437	H	3.578376	-2.540620	-0.279247
O	4.293516	0.234870	-2.303090	H	-0.420105	3.370488	-2.726763
O	-0.397852	4.116152	-2.114350	H	-2.477744	-0.147709	2.934539
O	-2.278332	3.891823	0.174589	H	4.624111	-0.522507	1.018672
O	-1.522757	-0.099962	3.010243	H	1.199597	4.037113	-0.860942
O	0.459899	-2.020003	3.940953	H	-0.501395	1.426008	3.802655
H	-3.282114	-2.897835	0.263058	H	-1.626934	-0.089753	-1.933186
H	-1.322650	-4.047238	-0.647273	H	0.064094	-4.899039	-2.672571
H	-0.041357	-3.376021	-2.743474	H	-4.772030	-3.162830	0.401002
H	-0.998102	-1.527460	-3.715370	H	-5.087447	2.636888	0.426007
H	-3.011885	-0.158102	-2.549951	H	0.466508	-4.896179	2.648140
H	-4.544449	-0.998800	-1.022533	H	1.205111	0.080489	-2.106603
H	-4.345333	0.527697	1.731540	H	5.087531	-2.636901	-0.425786
H	1.760152	-3.900763	0.627585	H	-0.466681	4.896328	-2.648454
H	0.329614	1.499529	-3.798489	H	-1.205029	-0.080415	2.106912
H	4.544236	0.998819	1.022491	H	4.771956	3.162826	-0.400926
H	3.282018	2.897814	-0.263293	H	-0.063995	4.898897	2.672320
H	1.322590	4.047135	0.647004	H	1.626911	0.089715	1.933493

Isomer: n=24 ($4^6 6^8$B) Geometry: B3LYP/6-31+G(d)-6-311+2+G(d,p++)

	X	Y	Z
O	-4.541535	0.207833	-1.281665
O	-2.079940	0.118639	-2.419379
O	-0.608845	-1.872165	-3.736106
O	-0.445823	-3.867624	-2.005984
O	-2.165728	-3.683347	0.246864
O	-4.198594	-1.946304	0.560561
O	-4.026330	2.291596	0.602652
O	-4.010237	0.150527	2.493542
O	0.110407	-3.928133	1.923941
O	1.842542	-3.848901	-0.325209
O	1.326783	-0.020513	-2.903427
O	-0.446592	1.997949	-3.708360
O	4.535458	-0.207531	1.276648
O	4.195750	1.946920	-0.565963
O	2.159026	3.679126	-0.254833
O	0.440307	3.863691	1.997242
O	0.610467	1.877347	3.737836
O	2.075579	-0.117338	2.418955
O	4.019319	-2.290052	-0.609180
O	4.008586	-0.148629	-2.499488
O	-0.117115	3.932045	-1.932718
O	-1.848316	3.848095	0.317906
O	-1.328840	0.029322	2.905485
O	0.439662	-1.996690	3.702162
H	-3.387432	-2.525409	0.436932
H	-1.675617	-3.686659	-0.606497
H	-0.510479	-3.116309	-2.677646
H	-1.312403	-1.273039	-3.392793
H	-3.032768	0.154115	-2.123752
H	-4.481501	-0.581867	-0.699675
H	-4.053639	0.939319	1.908914
H	1.353646	-3.824678	0.528517
H	0.323490	1.393835	-3.591503
H	4.475652	0.582421	0.694984
H	3.383251	2.524586	-0.444053
H	1.667560	3.679457	0.597815
H	0.507701	3.116131	2.672714
H	1.312203	1.276422	3.393816
H	3.027760	-0.153204	2.121456
H	4.050872	-0.937754	-1.915212
H	-1.360033	3.825681	-0.536184
H	-0.329001	-1.390390	3.587012
H	-4.418199	0.978587	-0.684491
H	0.208342	-1.336004	-3.607723
H	-1.454538	-3.704564	0.926921
H	-3.169193	2.802578	0.489290
H	0.237614	-3.201288	2.613379
H	2.323556	-0.069651	-2.886421
H	4.117422	0.622527	-1.900052
H	-1.138020	3.794126	0.997027
H	1.191935	-1.452665	3.370468
H	-4.116995	-0.621091	1.894377
H	1.132585	-3.798061	-1.004872
H	-1.197412	1.453530	-3.374138
H	3.162058	-2.800909	-0.496601
H	-0.244959	3.206076	-2.622820
H	-2.325611	0.075877	2.885423
H	4.410664	-0.977823	0.679215
H	1.449077	3.702970	-0.935948
H	-0.207832	1.342022	3.613476
H	-1.570049	0.091522	-1.579404
H	-0.546840	-4.689545	-2.511252
H	-4.938549	-2.566296	0.656278
H	-4.712321	2.969081	0.709865
H	0.140697	-4.767425	2.409519
H	1.071827	-0.012922	-1.954056
H	4.705458	-2.967793	-0.713793
H	-0.146653	4.772093	-2.417006
H	-1.070725	0.027353	1.956865
H	4.935164	2.568125	-0.658017
H	0.543176	4.688365	2.497668
H	1.563984	-0.088969	1.579838
Bq	0.130572	0.031752	0.170055

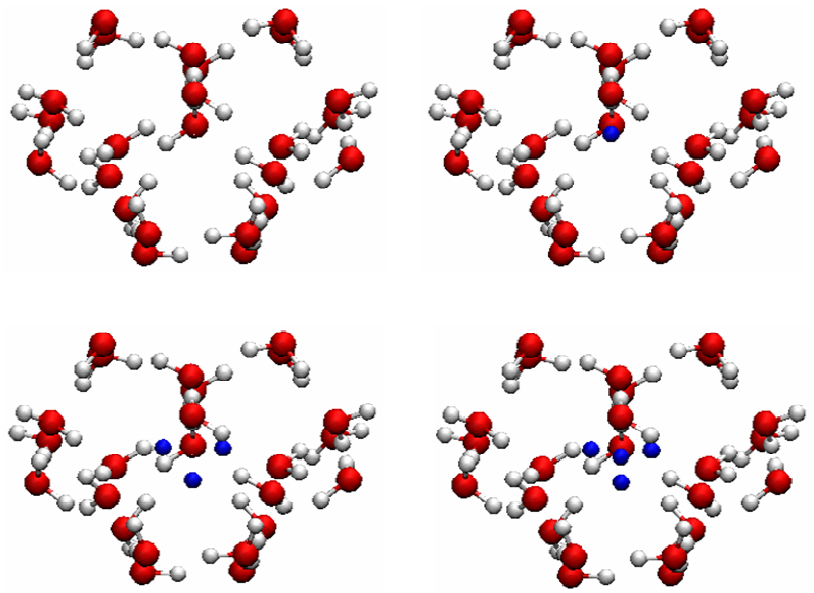


Figure S2. The geometric structures for isomer $5^{12}6^{2}$B with different number of additional ghost atoms (n=0,1,3,4). The blue circles denote the position where ghost atoms located.

2. The Calculated Electronic Properties for $5^{12}6^{2}$B with Additional Diffuse Functions

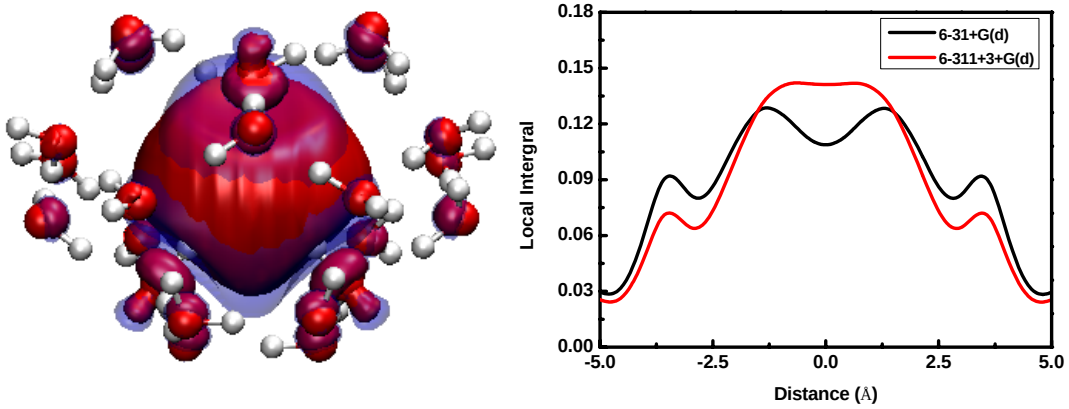


Figure S3. The spin density distributions (isovalue=0.004) and corresponding local integral along the z-axis for isomer $5^{12}6^{2}$B with different basis sets. The blue and red surfaces present the contour map at 6-31+G(d) and 6-311+3+G(d) basis set levels, respectively.

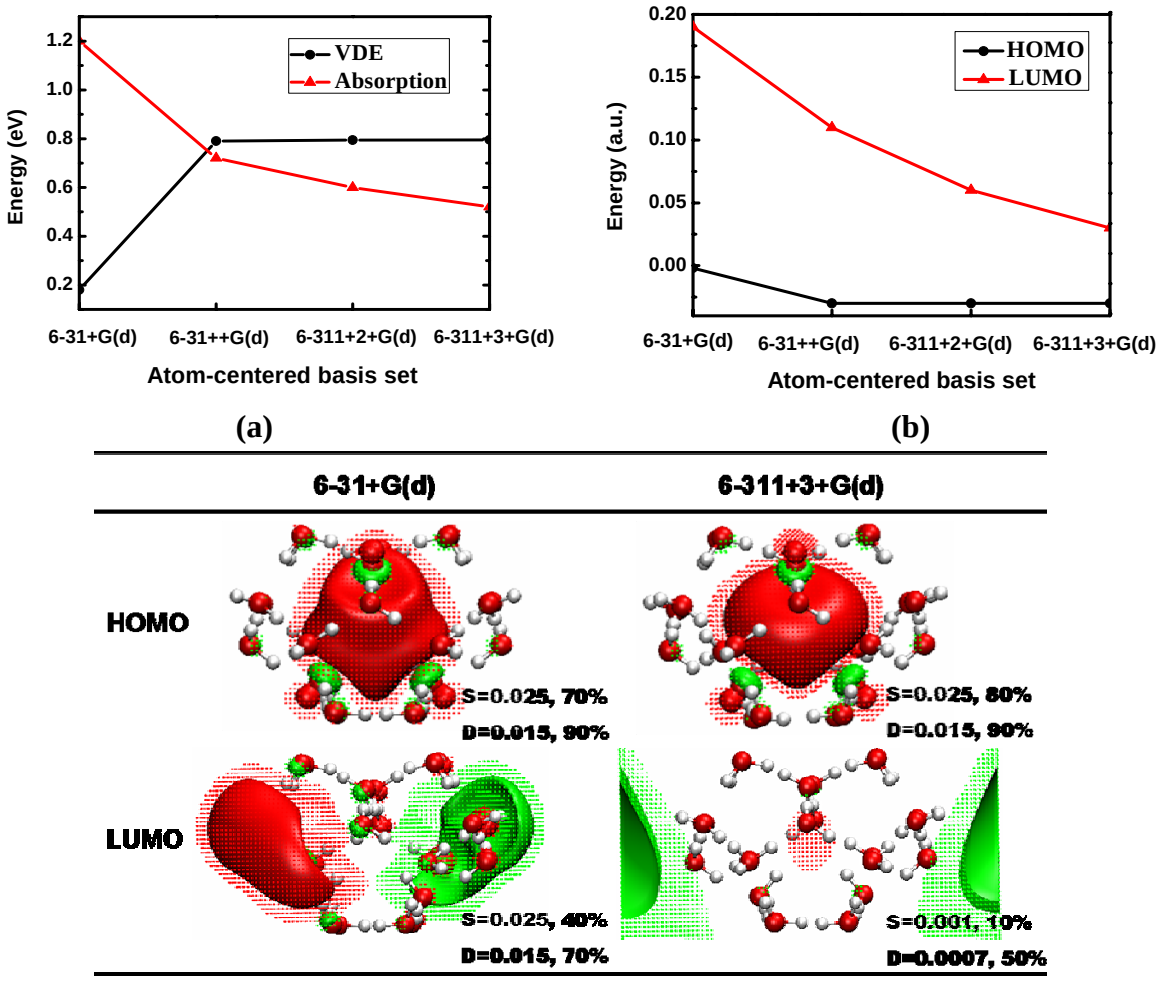


Figure S4. The calculated VDEs **(a)**, the HOMO and LUMO energies **(b)** and distributions **(c)** of the $(H_2O)_{24}^-$ $5^{12}6^2$B isomer at mp2 level. The vis absorption maxima at TDDFT/B3LYP level, with respect to different atom-centered basis sets are also shown in **(a)**.

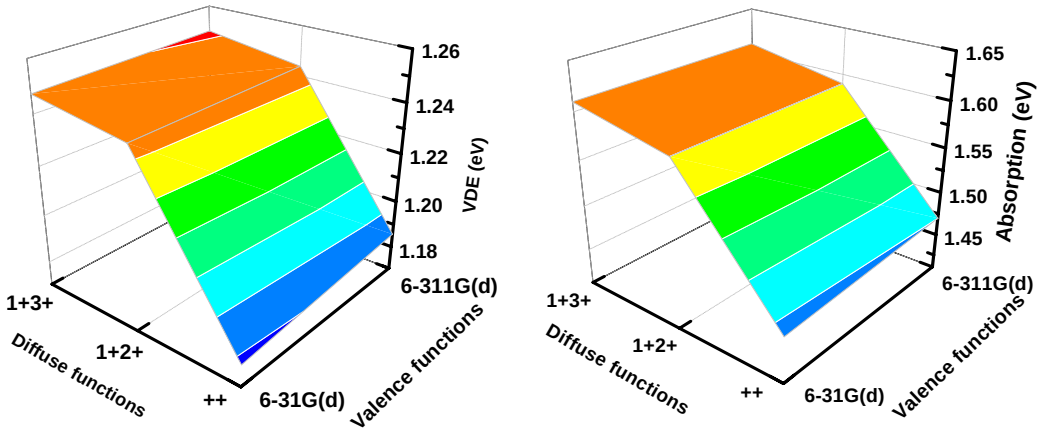


Figure S5. The calculated VDEs and vis absorption maxima for the $(H_2O)_{24}^-$ $5^{12}6^2$B isomer using a fixed atom-centered basis set [6-31+G(d)] at the B3LYP level for all H_2O molecules augmented by one H ghost atom with different ghost-atom-based diffuse and valence functions

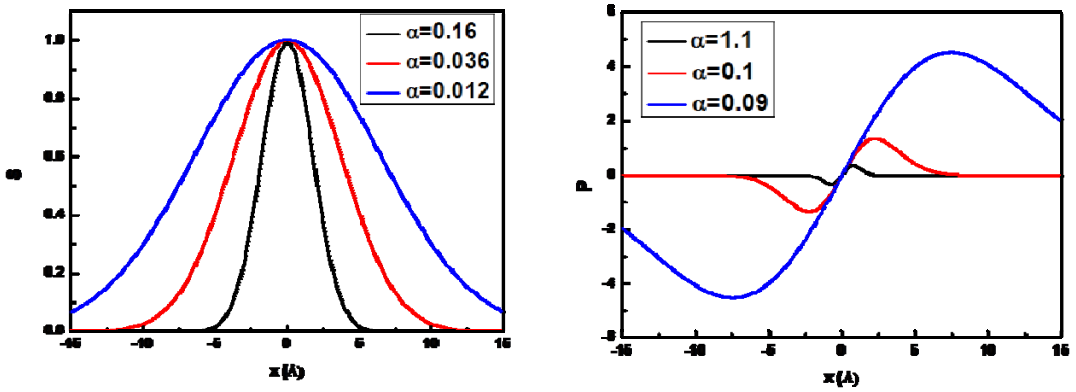
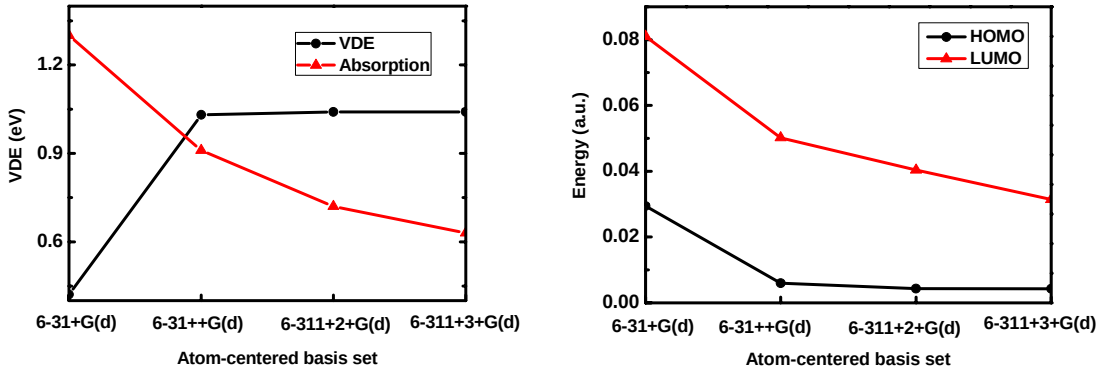


Figure S6. The employed s (left) and p (right) diffuse functions with different orbital coefficients. The s and p diffuse functions are given as $s = e^{-\alpha \bullet x^2}$ and $p = x \bullet e^{-\alpha \bullet x^2}$, respectively, where α denotes the orbital coefficients.

3. The Calculated Electronic Properties for Isomer $4^6 6^8$B with Additional Diffuse Functions



A **B**

Figure S7. Calculated VDEs, vis absorption maxima (**A**), and the HOMO and LUMO energies (**B**) of the $(H_2O)_{24}^-$ $4^6 6^8$B isomer, with respect to different atom-centered basis sets at the B3LYP level.

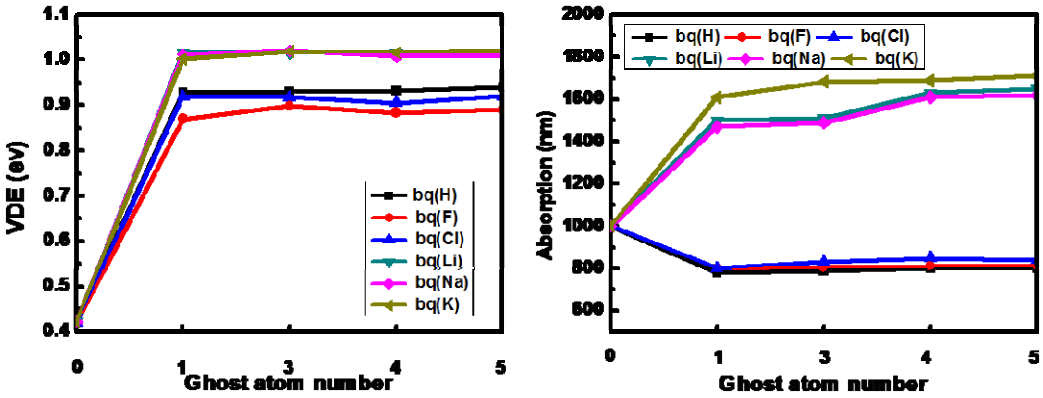
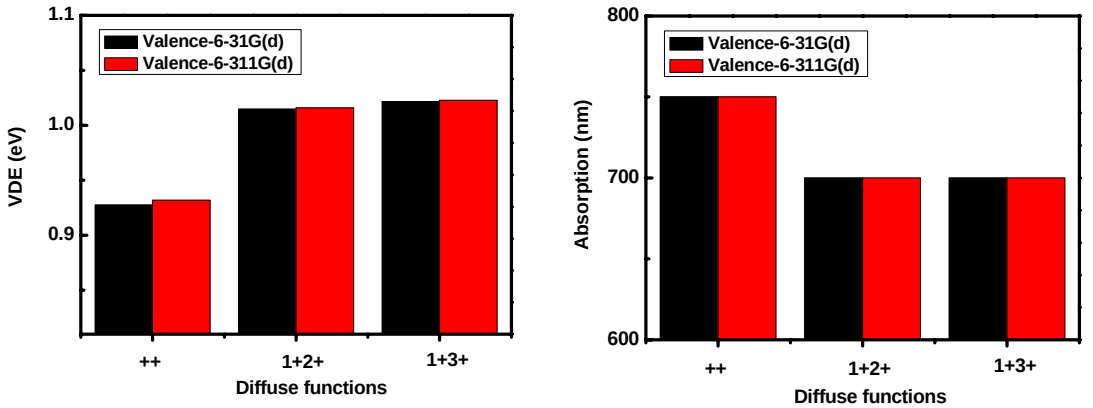
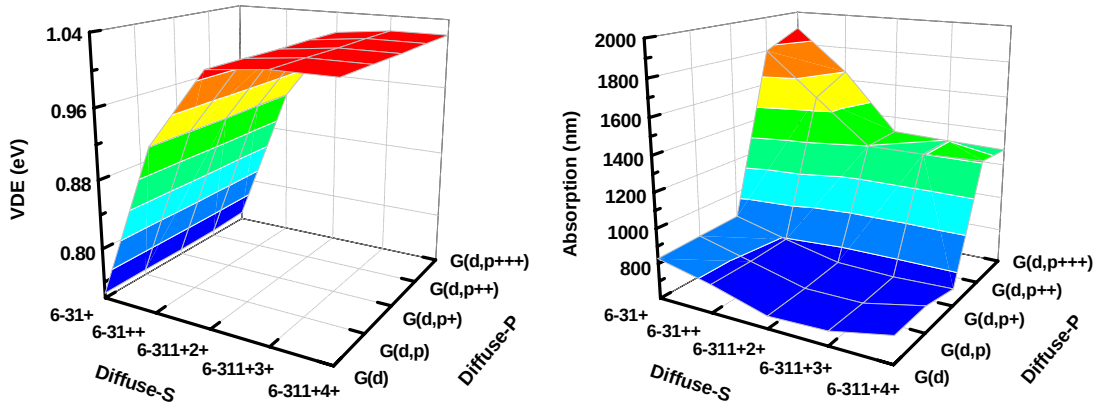


Figure S8. The VDEs, vis absorption maxima for isomer $(H_2O)_{24}^-$, and their dependence on the number and kinds of ghost atoms at the B3LYP level. The solid lines depict the results with low-quality atom-centered basis set [6-31+G(d)] augmented by ghost atoms at the 6-31++G(d) level. The considered ghost atom is H, F, Cl, Li, Na, and K atom, respectively.



A **B**

Figure S9. The VDEs (**A**) and vis absorption maxima (**B**) for the $(H_2O)_{24}^-$ $4^6 6^8$B isomer at the B3LYP level using fixed atom-centered basis set [6-31+G(d)] augmented by one H ghost atom with different ghost-atom-based diffuse and valence functions.



A **B**

Figure S10. Calculated VDEs and vis absorption maxima for the $(H_2O)_{24}^-$ $4^6 6^8$B isomer at the B3LYP level using 6-31+G(d) atom-centered basis set augmented by one H ghost atom with different ghost-atom-based diffuse functions.

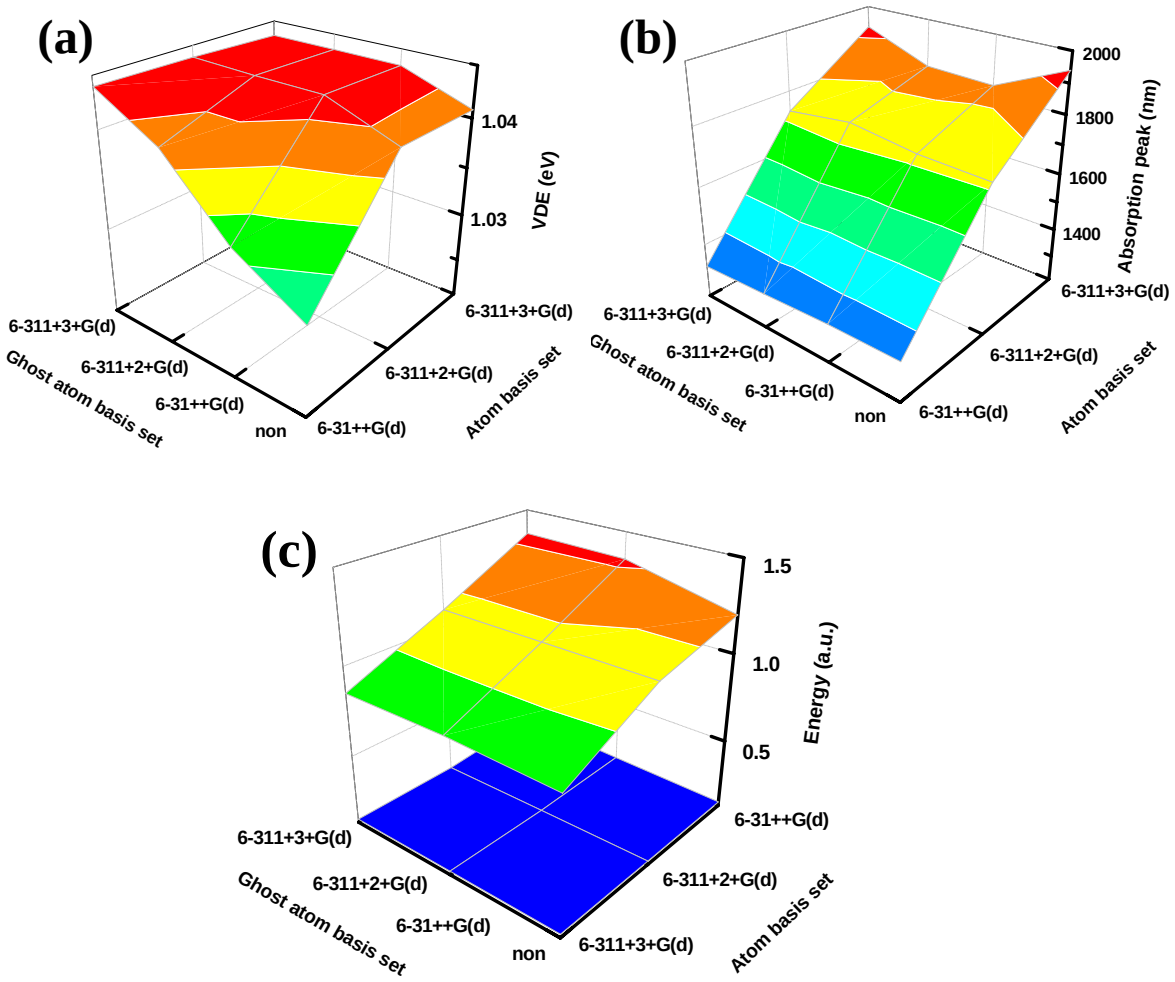
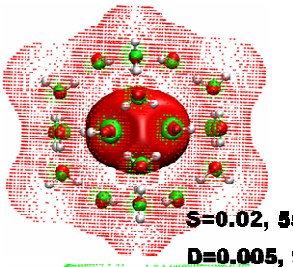
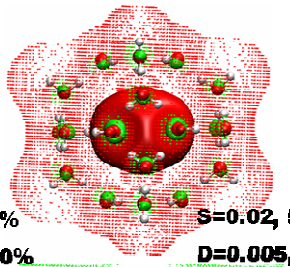
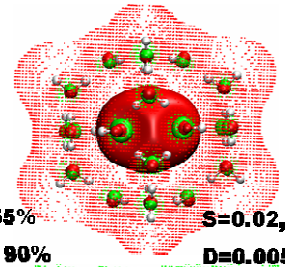
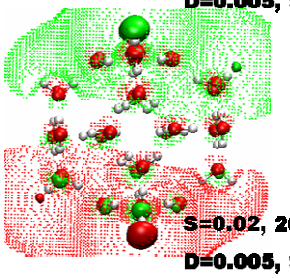
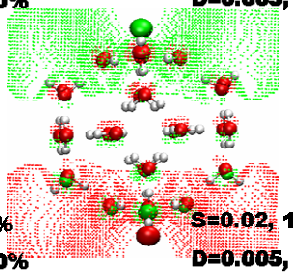
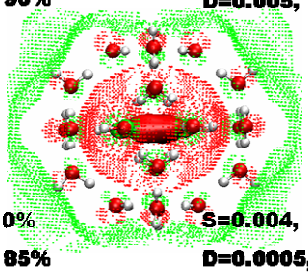
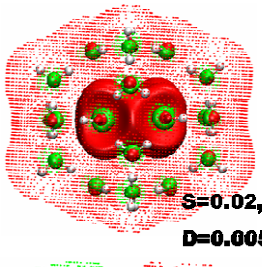
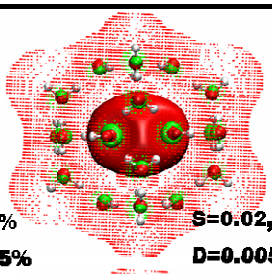
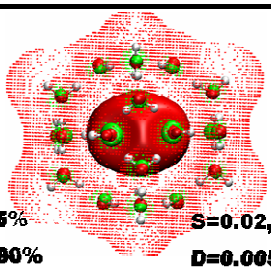


Figure S11. Calculated VDEs **(a)**, vis absorption maxima **(b)** and HOMO/LUMO energies **(c)** for the $(H_2O)_{24}^-$ $4^6 6^8$B isomer, with respect to different basis sets at the B3LYP level. One H is selected as additional ghost atom.

Table S2. HOMO and LUMO Distributions for the isomer $4^6 6^8$B at the B3LYP level with different basis sets. The solid (S) and dotted (D) surface present the contour map with different isovalues. The detailed data and the density enclosed in the surface are both shown in the right bottom.

	6-31++G(d)	6-311+2+G(d)	6-311+3+G(d)
HOMO			
LUMO			

	6-31+G(d)	6-31+G(d)-bq(H)-6-311+2+G(d)	6-31+G(d)-bq(H)-6-311+2+G(d,p++)
HOMO			
LUMO