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

Efficient Floating Diffuse Functions for Accurate Characterization of the Surface-Bound Excess Electrons in Water Cluster Anions

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Supporting Information

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1. The Calculated Structures and Electronic Properties for the $(H_2O)_{12}^-$ Cub Isomer with Additional Diffuse Functions

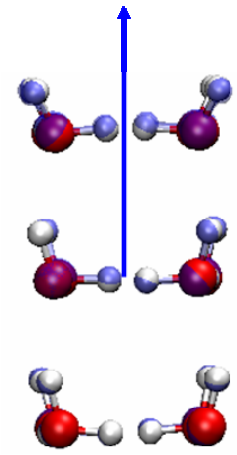


Figure S1. The optimized structures for isomer Cub of $(H_2O)_{12}^-$ at different levels. The solid structure is optimized at the MP2/6-31++G(d) level and the blue one is optimized at the MP2/6-31+3+G(d) level. The blue arrow denotes the vector of the dipole moment (μ). The corresponding coordinates in angstrom and dipole moments in debye are given in Table S1.

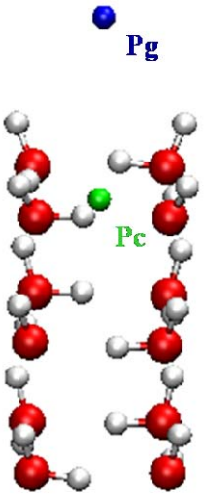


Figure S2. The optimized structure for isomer Cub of $(H_2O)_{12}^-$. The Pg denotes the position of the ghost atom and the Pc denotes the center of the nearby four oxygen atoms in the top layer of $(H_2O)_{12}^-$. The corresponding coordinates in angstrom is given in Table S2.

Table S1. The structure coordinates for Cub of $(H_2O)_{12}^-$. The unit is in Å.

Geometry: MP2/6-31++G(d)				**μ =22.5 D**			
	X	Y	Z		X	Y	Z
O	1.154192	1.552681	-3.639748	O	-0.774272	3.575901	-3.843947
H	0.521077	0.790534	-3.618018	H	-0.012427	2.943605	-3.799573
H	1.474152	1.637102	-2.715798	H	-0.807733	3.988418	-2.954061
O	-0.824702	-0.147603	-0.681244	O	-0.878234	-0.374136	-3.536390
H	-0.065017	0.492939	-0.638420	H	-0.887958	-0.642761	-2.592497
H	-0.836289	-0.588502	0.193304	H	-1.638996	0.254543	-3.626823
O	1.084496	1.896896	-0.796722	O	-0.668506	-0.626502	-6.428917
H	1.572648	1.971383	0.049161	H	0.084474	0.002732	-6.550409
H	0.447684	2.660912	-0.796496	H	-0.657209	-0.841181	-5.474184
O	-0.962197	3.797014	-0.994046	O	1.247657	1.466315	-6.548053
H	-0.989932	4.368899	-0.199353	H	1.514390	1.573106	-5.612543
H	-1.725402	3.168196	-0.887486	H	0.613122	2.206922	-6.710967
O	-2.871399	1.752517	-0.878560	O	-0.847491	3.373274	-6.747071
H	-2.238110	1.000222	-0.729408	H	-0.902677	3.734184	-5.839092
H	-3.398876	1.809043	-0.055194	H	-1.596264	2.730025	-6.804051
O	-2.806703	1.649077	-3.740586	O	-2.763644	1.280458	-6.627928
H	-3.169833	1.708571	-2.830759	H	-2.124905	0.525841	-6.643492
H	-2.172511	2.407615	-3.808370	H	-3.074239	1.319889	-5.700725

Geometry: MP2/6-311+3+G(d)				**μ =22.2 D**			
	X	Y	Z		X	Y	Z
O	0.005804	-0.023639	0.010400	O	-0.728811	2.653028	-0.331231
H	-0.004900	-0.021949	1.001550	H	-0.500041	1.688594	-0.326097
H	0.957159	-0.031510	-0.227620	H	0.097432	3.102722	-0.608519
O	2.769565	1.007336	2.662440	O	-0.023978	0.322294	2.785352
H	2.898435	0.828354	1.694364	H	0.927286	0.355143	3.021590
H	3.637295	0.838750	3.078620	H	-0.314515	1.269959	2.781642
O	2.765164	0.786311	-0.124450	O	-2.805526	-0.560588	2.783661
H	3.626620	0.570735	-0.531885	H	-2.865259	-0.760063	1.816860
H	2.603140	1.743408	-0.333091	H	-1.845420	-0.526560	2.968110
O	2.030225	3.475255	-0.336547	O	-2.826724	-0.723564	-0.047804
H	2.674918	4.054445	-0.787650	H	-1.879266	-0.679028	-0.287225
H	2.092464	3.706099	0.627119	H	-3.169640	0.187424	-0.222648
O	2.034636	3.696277	2.450332	O	-3.572066	2.008776	-0.199501
H	2.387768	2.791070	2.654571	H	-2.735424	2.462577	-0.425499
H	2.685589	4.322472	2.822788	H	-3.682750	2.161980	0.771241
O	-0.758569	2.998967	2.443734	O	-3.550846	2.171752	2.631964
H	0.067586	3.489356	2.640650	H	-3.378360	1.214492	2.810747
H	-0.809635	2.980530	1.454014	H	-2.701544	2.615036	2.829870

Table S2. The structure coordinates for Cub of $(H_2O)_{12}^-$. The unit is in Å.

Geometry: MP2/6-31++G(d)				μ =22.5 D			
	X	Y	Z		X	Y	Z
O	-0.093560	1.851469	-0.714873	O	-0.091515	0.719791	1.847618
H	-0.113649	0.998472	-1.218997	H	-0.117035	1.223784	0.994689
H	0.823407	2.183295	-0.822653	H	0.825914	0.832510	2.176515
O	2.782309	-0.594009	-1.881223	O	-0.081342	-0.710993	-1.846550
H	2.855774	0.335490	-1.537840	H	0.837743	-0.815831	-2.173425
H	3.627135	-0.759816	-2.346468	H	-0.104415	-1.215194	-0.993674
O	2.770229	1.901592	-0.607047	O	-2.991997	-0.604316	-1.919411
H	3.612009	2.371369	-0.775543	H	-3.086401	0.318021	-1.575755
H	2.848497	1.558627	0.322215	H	-2.058076	-0.665443	-2.204843
O	2.772959	0.627422	1.888579	O	-3.004209	1.908689	-0.598888
H	3.615310	0.800445	2.355679	H	-2.072034	2.199129	-0.662997
H	2.855132	-0.301411	1.545362	H	-3.093822	1.564548	0.323746
O	2.785057	-1.868171	0.614410	O	-3.001298	0.588165	1.914144
H	2.862411	-1.524539	-0.314682	H	-2.068557	0.657295	2.201603
H	3.630470	-2.330707	0.784747	H	-3.087043	-0.334944	1.570292
O	-0.079285	-1.842670	0.715939	O	-2.989081	-1.924839	0.593620
H	0.840261	-2.166608	0.825726	H	-3.079620	-1.581470	-0.329211
H	-0.107799	-0.989882	1.220010	H	-2.054595	-2.207287	0.659770
				H-bq	6.738661	0.032981	0.007902

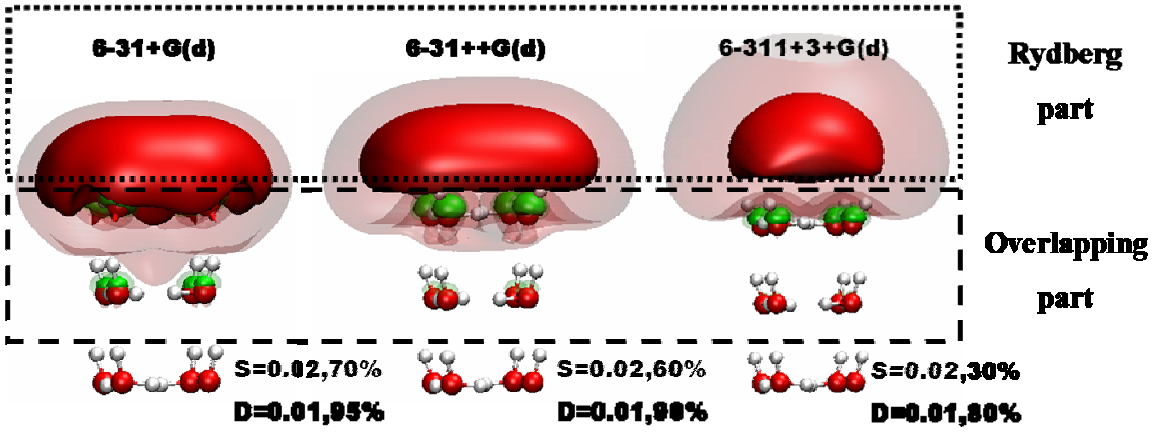


Figure S3. The HOMO distributions for the $(H_2O)_{12}^-$ Cub isomer, with respect to different atom-centered basis sets at the MP2 level. The solid (S) and dotted (D) surface present the contour map with different isovalues. The detailed data and the density enclosed in the surface are both shown in the right bottom.

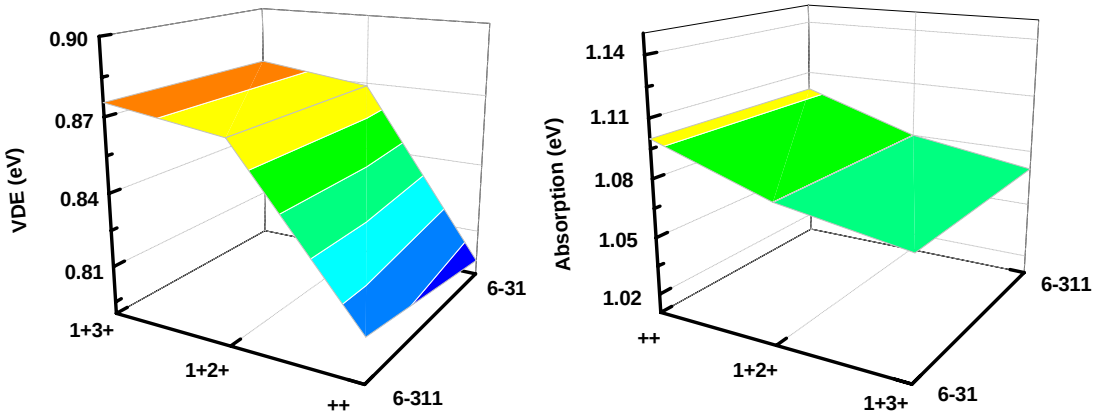
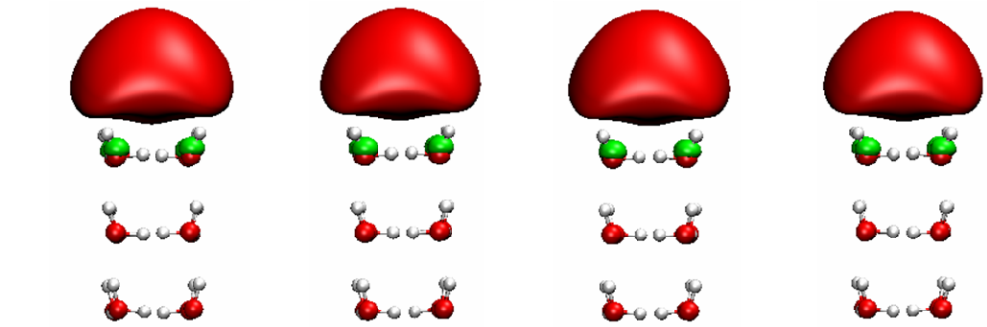
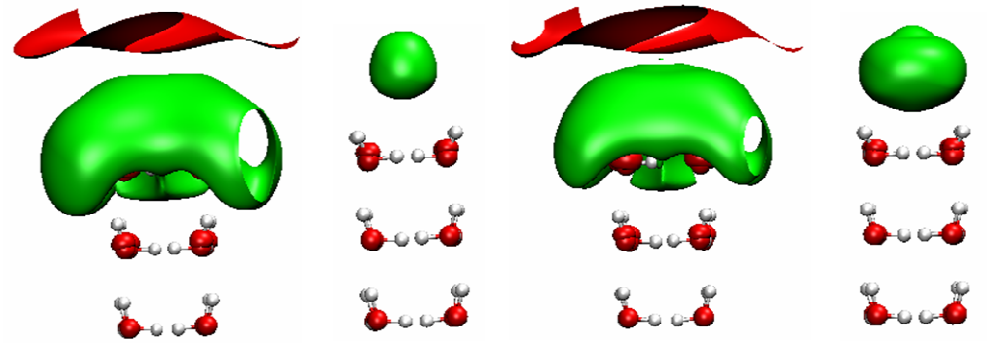


Figure S4. The calculated VDEs (at the MP2 level) and UV absorption maxima (at the TDDFT/B3LYP level) for the $(H_2O)_{12}^-$ Cub isomer using a fixed atom-centered basis set [6-31++G(d)] for all H_2O molecules augmented by one H ghost atom with different ghost-atom-based diffuse and valence functions.

Table S3. The HOMO (i.e. SOMO, isovalue=0.02) and LUMO (isovalue=0.01) distributions for the quadrangular $(H_2O)_{12}^-$ Cub isomer, with respect to different atom-centered basis sets at the MP2 level.

Cub	**6-31++G(d)-bq(H)-6-311+2+G(d)**	**6-31++G(d)-bq(H)-6-311+3+G(d)**	**6-31++G(d)-bq(H)-6-3111+2+G(d)**	**6-31++G(d)-bq(H)-6-3111+3+G(d)**
HOMO				
LUMO				

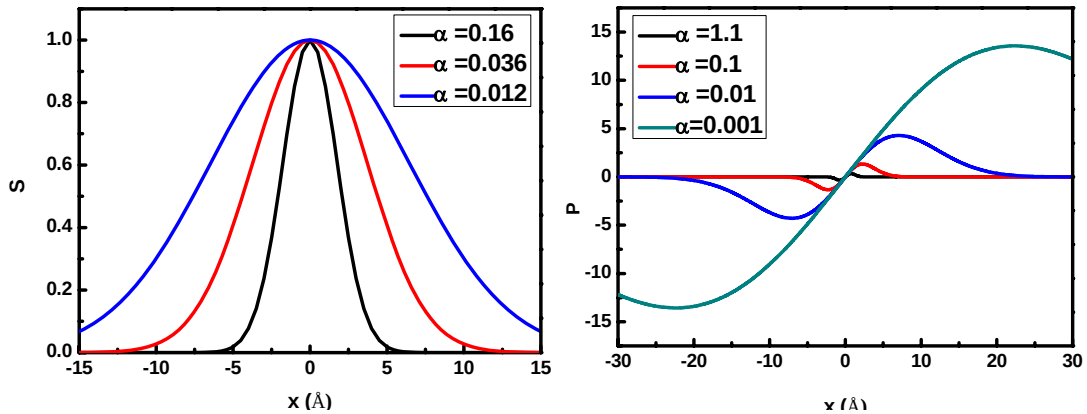


Figure S5. The employed s (left) and p (right) diffuse functions with different orbital exponents. The s and p diffuse functions are given as $s = e^{-\alpha \bullet x^2}$ and $p = x \bullet e^{-\alpha \bullet x^2}$, respectively, where α denotes the orbital exponents.

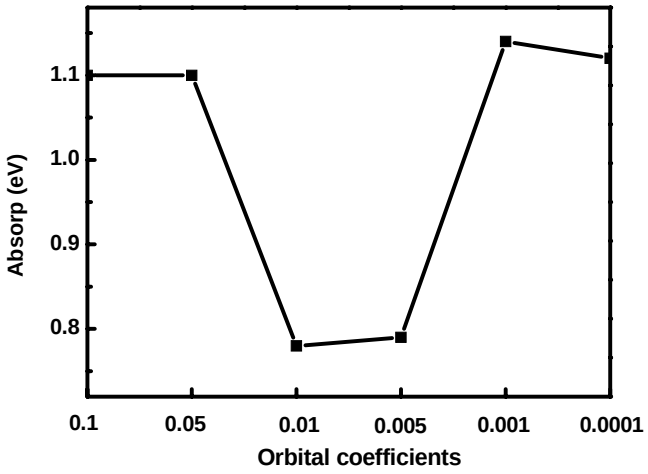


Figure S6. The dependence of the UV absorption maxima on the orbital exponents in the basis sets calculated at the TDDFT/B3LYP level.

Table S4. The LUMO distributions for the isomer Cub at the MP2 level with different basis sets. The values in parentheses are the smallest p-orbital exponents. 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.

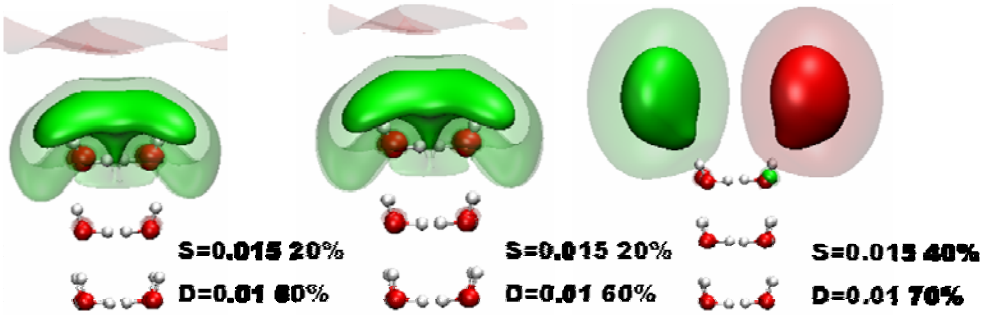
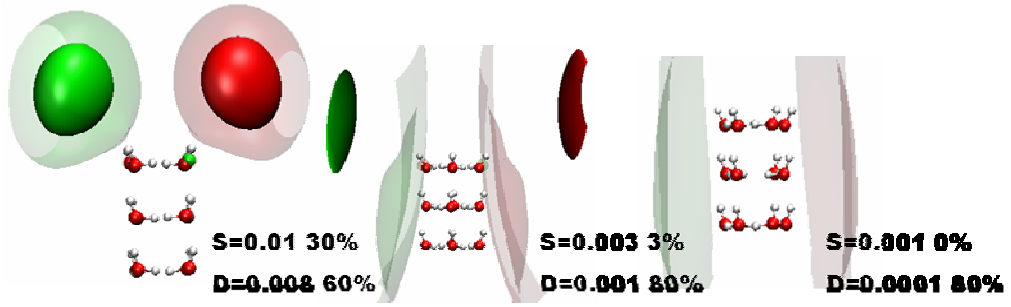
Cub	6-31++G(d)-bq(H)-6-311+2+G(d,p++) (0.1)	6-31++G(d)-bq(H)-6-311+2+G(d,p++) (0.05)	6-31++G(d)-bq(H)-6-311+2+G(d,p++) (0.01)
LUMO			
Cub	**6-31++G(d)-bq(H)-6-311+2+G(d,p++) (0.005)**	**6-31++G(d)-bq(H)-6-311+2+G(d,p++) (0.001)**	**6-31++G(d)-bq(H)-6-311+2+G(d,p++) (0.0001)**
LUMO			

Table S5. The calculated VDEs of the $(H_2O)_{12}^-$ isomer with different basis sets.

VDE(eV)	6-31++G(d)	6-311+3+G(d)	6-31++G(d)-bq(H)-6311+2+G(d,p++)
MP2	0.69	0.79	0.88
CCSD	0.70	0.81	0.91

Table S6. The HOMO and LUMO distributions for the $(H_2O)_{12}^-$ isomer calculated using different basis sets at the CCSD level.

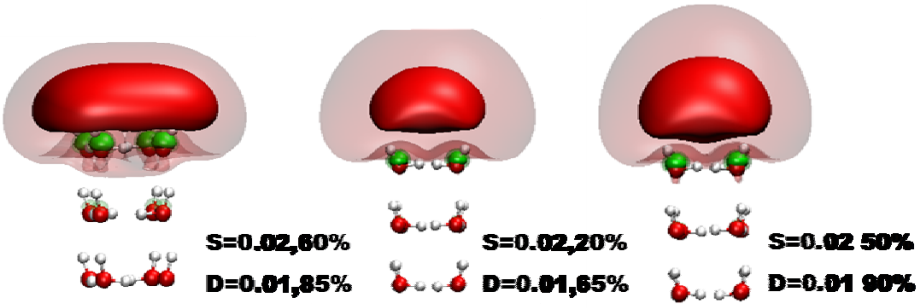
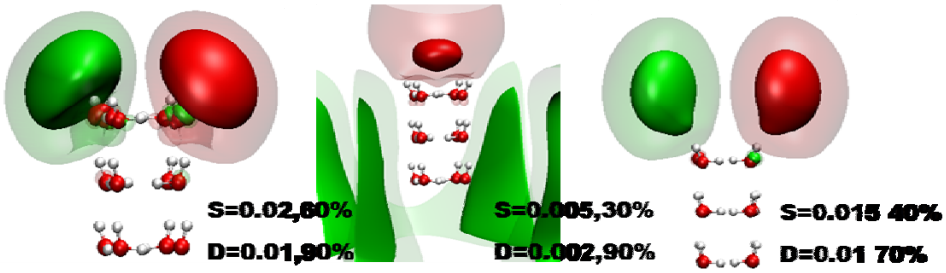
$(H_2O)_{12}^-$	**6-31++G(d)**	**6-311+3+G(d)**	**6-31++G(d)-bq(H)-6311+2+G(d,p++)**
HOMO			
LUMO			

Table S7. The calculated UV maxima of the $(H_2O)_{12}^-$ isomer with different basis sets.

Absorption Peak (eV)	6-31++G(d)	6-311+3+G(d)	6-31++G(d)-bq(H)-6311+2+G(d,p++)
B3LYP	1.0	0.68	0.78
X3LYP	1.0	0.68	0.79
CAM-B3LYP	0.93	0.67	0.76
M062X	0.96	0.69	0.78

2. The Calculated Structures and Electronic Properties for the $(5^{12})^{-}$A Isomer of $(H_2O)_{20}^{-}$ with Additional Diffuse Functions

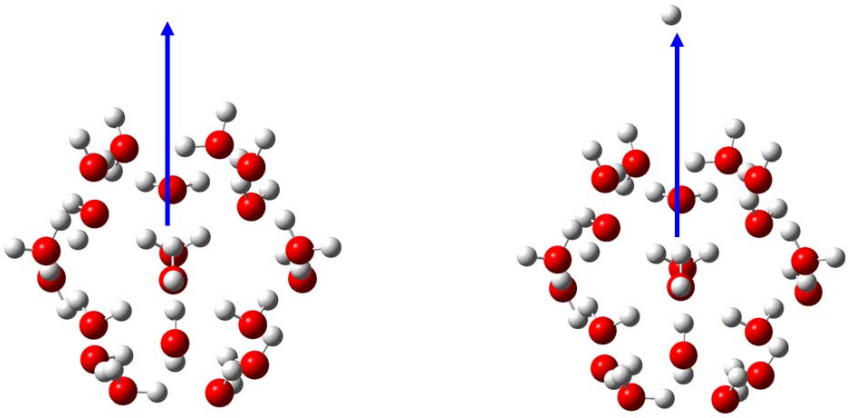


Figure S7. The optimized structures for isomer $(5^{12})^{-}$A of $(H_2O)_{20}^{-}$ at different levels. The left structure is optimized at the B3LYP/6-311+3+G(d) level and the right one is optimized at the B3LYP/6-31++G(d)-bq(H)-6-31++G(d) level. The blue arrow denotes the vector of the dipole moment (μ). The corresponding coordinates in angstrom and dipole moments in debye are given in Table S5.

Table S8. The structure coordinates for $(5^{12})^{-}$A of $(H_2O)_{20}^{-}$. The unit is in Å.

Geometry: B3LYP/6-311+3+G(d)				**μ =28.9 D**			
	X	Y	Z		X	Y	Z
O	0.107328	1.485649	-3.509828	O	-2.069060	-3.477575	-0.136874
H	-0.071363	0.475031	-3.546596	H	-2.207669	-2.995971	0.705378
H	0.139931	1.780207	-4.434035	H	-2.304658	-2.840720	-0.839261
O	-1.790856	2.645188	-1.946482	O	0.754057	-3.925885	-0.428579
H	-1.106901	2.254564	-2.566292	H	-0.213506	-3.821016	-0.296366
H	-2.191983	3.409920	-2.413609	H	1.181574	-3.616933	0.410207
O	-0.658450	3.731588	0.319231	O	1.962772	-2.987141	1.907206
H	-1.058574	3.323923	-0.498699	H	1.313201	-2.586198	2.525190
H	-0.951083	4.670079	0.295464	H	2.614259	-2.275170	1.705464
O	-1.681331	2.491155	2.554545	O	3.765909	-0.902909	1.237556
H	-1.319420	2.945174	1.745616	H	3.504179	-0.038554	1.627109
H	-2.197013	3.174886	3.018459	H	3.683199	-0.786889	0.269028
O	0.440471	1.116413	3.741839	O	2.884359	1.599802	2.285330
H	-0.321550	1.637978	3.392440	H	2.051397	1.421326	2.767337
H	0.545235	1.372570	4.670750	H	2.638278	2.197023	1.550613
O	-0.006818	-1.762155	3.606599	O	2.083193	3.361427	0.119429
H	0.161090	-0.799562	3.619990	H	1.112093	3.540341	0.199776
H	-0.862875	-1.869363	3.142018	H	2.513927	4.231182	0.134945
O	-2.537388	-1.998115	2.272575	O	2.623259	1.896551	-2.268571
H	-2.890339	-1.092780	2.042810	H	1.752511	1.770667	-2.707611
H	-3.207045	-2.410381	2.838356	H	2.440952	2.409335	-1.451756
O	-3.474682	0.454217	1.655779	O	3.553491	-0.559622	-1.621724
H	-3.556792	0.587744	0.686497	H	3.235194	0.355062	-1.861865
H	-2.865174	1.156676	1.970886	H	4.418860	-0.664142	-2.043936
O	-3.694513	0.818892	-1.174251	O	1.624403	-2.466147	-2.561780
H	-3.018112	1.490390	-1.461529	H	1.319393	-3.022287	-1.790976
H	-4.556688	1.219938	-1.385231	H	2.299112	-1.854527	-2.200691
O	-2.824374	-1.601178	-2.245036	O	-0.374694	-1.054843	-3.636085
H	-3.208936	-0.759669	-1.899039	H	-1.187762	-1.294858	-3.145249
H	-3.497991	-1.996060	-2.819234	H	0.369297	-1.609750	-3.245079

Geometry: B3LYP/6-31++G(d)-bq(H)-6-31++G(d) μ=29.1 D

	X	Y	Z
O	0.095522	1.490458	-3.491526
H	-0.080374	0.480095	-3.540693
H	0.111598	1.802004	-4.410802
O	-1.796533	2.608361	-1.890861
H	-1.118287	2.238598	-2.529228
H	-2.213994	3.383269	-2.330055
O	-0.630450	3.707967	0.343514
H	-1.040548	3.289308	-0.464893
H	-0.937555	4.643476	0.316671
O	-1.655787	2.458011	2.564026
H	-1.293012	2.917994	1.757244
H	-2.176142	3.137559	3.029870
O	0.456792	1.084517	3.755471
H	-0.303630	1.602481	3.395296
H	0.558888	1.354940	4.680852
O	0.018174	-1.794022	3.627765
H	0.184553	-0.830801	3.642122
H	-0.832363	-1.903308	3.152895
O	-2.494495	-2.041356	2.269722
H	-2.849497	-1.132064	2.056024
H	-3.160704	-2.464599	2.831780
O	-3.445744	0.410797	1.683836
H	-3.538775	0.538041	0.714063
H	-2.836231	1.118893	1.987883
O	-3.684809	0.773030	-1.139970
H	-3.003138	1.443992	-1.421437
H	-4.544569	1.186020	-1.339891
O	-2.817991	-1.622660	-2.245159
H	-3.209419	-0.790620	-1.882206
H	-3.490829	-2.018397	-2.819890
O	-2.054365	-3.499272	-0.154999
H	-2.185611	-3.019418	0.689882
H	-2.290108	-2.859490	-0.855296
O	0.765451	-3.941035	-0.443143
H	-0.203005	-3.835617	-0.313709
H	1.191430	-3.632298	0.396689
O	1.971230	-3.000094	1.895957
H	1.327630	-2.608903	2.526851
H	2.621362	-2.285226	1.697925
O	3.773298	-0.916897	1.237877
H	3.515979	-0.055998	1.638939
H	3.681373	-0.792189	0.270927
O	2.905071	1.577557	2.311716
H	2.071003	1.391974	2.790112
H	2.655624	2.166520	1.570852
O	2.107555	3.327540	0.139543
H	1.136955	3.514625	0.218770
H	2.547398	4.192508	0.171413
O	2.621910	1.892053	-2.271539
H	1.746264	1.768117	-2.702434
H	2.448898	2.401352	-1.449899
O	3.544594	-0.561962	-1.613750
H	3.228515	0.352381	-1.860348
H	4.409323	-0.674345	-2.035659
O	1.624700	-2.463176	-2.571470
H	1.323500	-3.025828	-1.803652
H	2.293517	-1.847462	-2.205530
O	-0.379688	-1.053396	-3.643471
H	-1.191302	-1.291776	-3.148823
H	0.365712	-1.605581	-3.250871
H-bq	-4.396811	6.233403	-0.850899

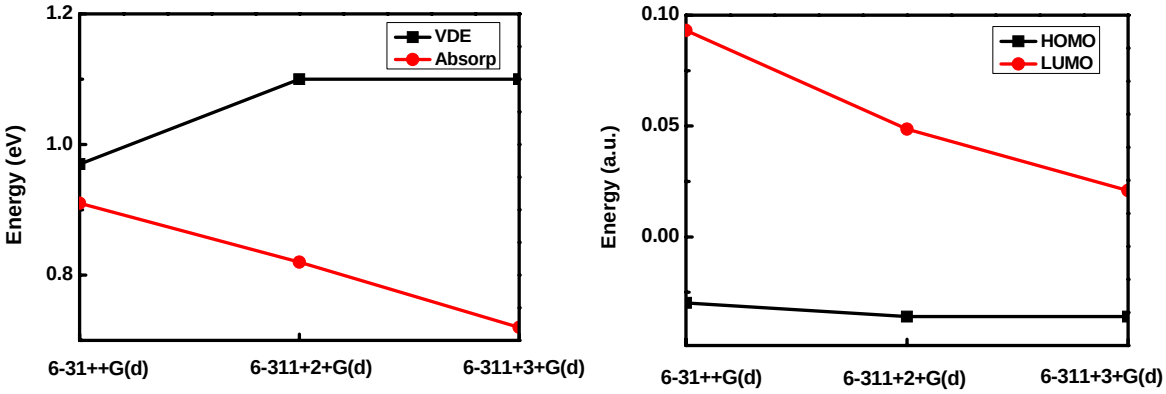
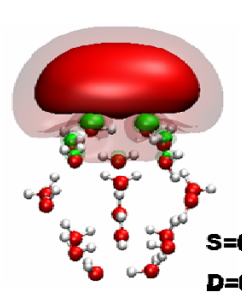
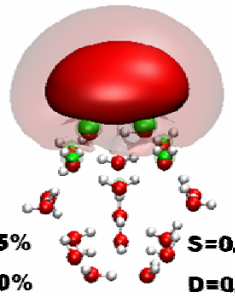
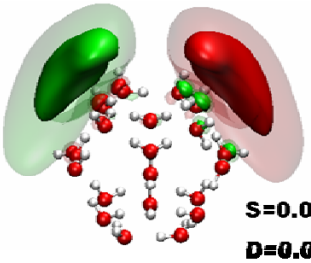
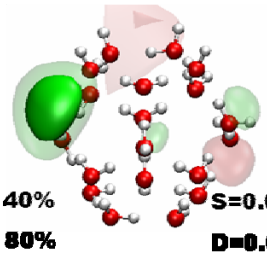


Figure S8. The calculated VDEs, the HOMO and LUMO energies of the $(H_2O)_{20}^-$ (5^{12}) $^-$A isomer, with respect to different atom-centered basis sets at the MP2 level. The UV absorption maxima shown in left are calculated at TDDFT/B3LYP level.

Table S9. HOMO and LUMO distributions for the isomer Cub at the MP2 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+3+G(d)
HOMO	 S=0.02 65% D=0.01 90%	 S=0.02 50% D=0.01 90%
LUMO	 S=0.02 40% D=0.01 80%	 S=0.0004 2% D=0.0003 10%

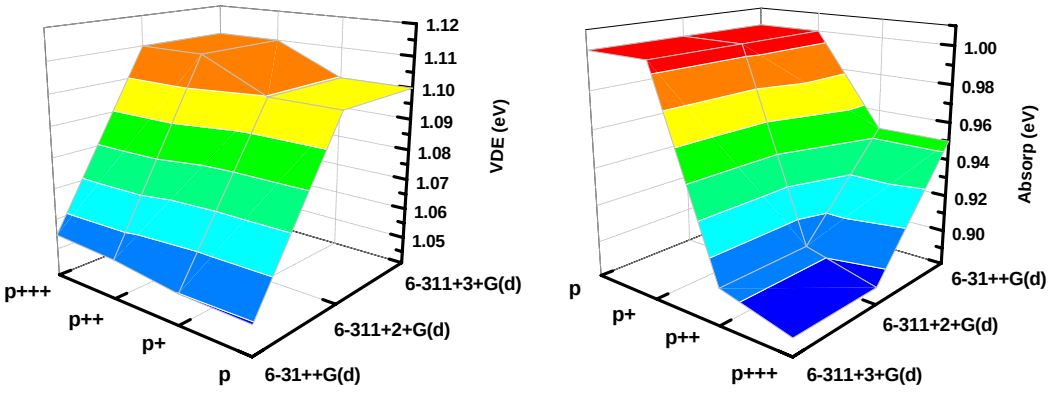
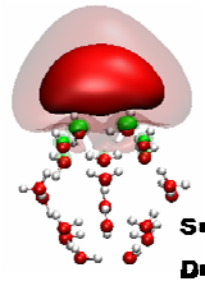
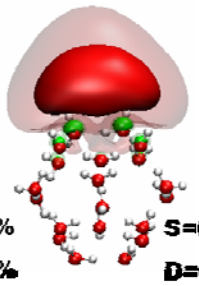
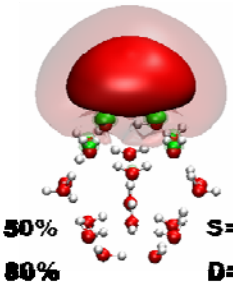
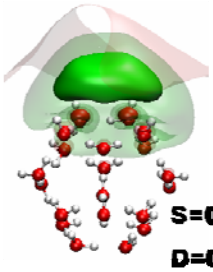
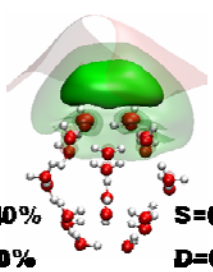
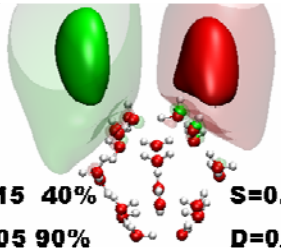


Figure S9. The calculated VDEs and UV absorption maxima for the $(H_2O)_{20}^-$ $(5^{12})^-$A isomer using 6-31++G(d) atom-centered basis set for all H_2O molecules augmented by one H ghost atom with different ghost-atom-based diffuse functions.

Table S10. The HOMO and LUMO Distributions for the $(H_2O)_{20}^-$ $(5^{12})^-$A isomer, with respect to different atom-centered basis sets at the MP2 level. 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.

Cub	6-31++G(d)-bq(H)-6-311+2+G(d,p)	6-31++G(d)-bq(H)-6-311+2+G(d,p+)	6-31++G(d)-bq(H)-6-311+2+G(d,p++)
HOMO	 S=0.02 50% D=0.01 80%	 S=0.02 50% D=0.01 80%	 S=0.02 50% D=0.01 80%
LUMO	 S=0.015 40% D=0.005 90%	 S=0.015 40% D=0.005 90%	 S=0.015 30% D=0.005 90%

3. The Calculated Structures and Electronic Properties for the $(H_2O)_{11}^-$ AA Isomer with Additional Diffuse Functions

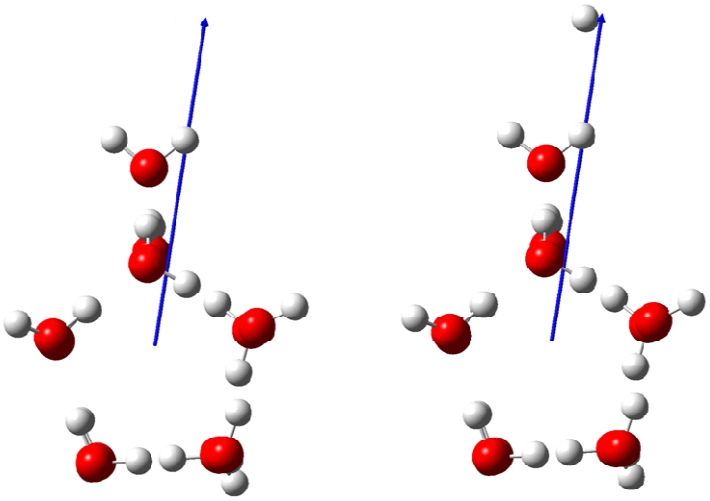


Figure S10. The optimized structures for $(H_2O)_{11}^-$ at different levels. The left structure is optimized at the B3LYP/6-311+3+G(d) level and the right one is optimized at the B3LYP/6-31++G(d)-bq(H)-6-31++G(d) level. The blue arrow denotes the vector of the dipole moment (μ). The corresponding coordinates in angstrom and dipole moments in debye are given in Table S5.

Table S11. The structure coordinates for $(H_2O)_{11}^-$. The unit is in Å.

Geometry: B3LYP/6-311+3+G(d) μ **=14.5 D**

	X	Y	Z		X	Y	Z
O	1.627665	0.982945	-3.64550000	H	-2.325785	3.351644	-3.91271500
H	1.193293	1.708697	-3.10893300	H	-2.055792	4.867716	-3.56151000
H	2.501993	0.846444	-3.24194300	O	-0.411606	-1.033087	-3.88745500
O	-1.247828	1.646044	-0.20946300	H	0.346537	-0.432290	-3.71449700
H	-0.807093	1.098731	0.48255900	H	-1.124561	-0.719547	-3.29036500
H	-1.891011	2.185695	0.30935000	O	-0.744973	-0.462529	-6.61166100
O	-2.484207	0.123965	-2.20856800	H	0.046139	0.130219	-6.68886100
H	-3.123617	-0.458961	-1.75849500	H	-0.698758	-0.789823	-5.67834600
H	-2.060746	0.638414	-1.47328700	O	1.269207	1.482633	-6.47950200
O	0.383267	2.921794	-2.23196500	H	1.503378	1.397684	-5.53030000
H	-0.285715	3.386134	-2.78636000	H	0.685222	2.275946	-6.53351800
H	-0.112688	2.573326	-1.45842000	O	-0.768433	3.471938	-6.59464000
O	-3.387928	2.047457	-4.10597600	H	-0.975898	3.835193	-5.70710500
H	-3.153270	1.331364	-3.47265600	H	-1.509499	2.857126	-6.78413400
H	-3.237781	1.686726	-5.01021200	O	-2.708051	1.319701	-6.74728100
O	-1.617515	4.062035	-3.88589100	H	-2.007547	0.589760	-6.72564800
				H	-3.346342	1.066048	-7.43515500

Geometry: B3LYP/6-31++G(d)-bq(H)-6-31++G(d) μ**=14.7 D**

	X	Y	Z		X	Y	Z
O	1.692347	1.041756	-3.791641	H	-1.996809	4.881414	-3.550768
H	1.294980	1.784562	-3.246877	O	-0.341830	-0.999795	-3.853642
H	2.584681	0.903856	-3.430750	H	0.412963	-0.381552	-3.736614
O	-0.921665	1.771467	-0.247760	H	-1.024581	-0.686919	-3.220132
H	-0.483319	1.196762	0.431161	O	-0.835836	-0.507389	-6.564408
H	-1.580104	2.277342	0.296738	H	-0.057965	0.090685	-6.705403
O	-2.296811	0.195220	-2.083362	H	-0.731913	-0.806283	-5.625591
H	-2.894885	-0.343363	-1.530554	O	1.160309	1.464838	-6.606204
H	-1.801925	0.748812	-1.419820	H	1.451452	1.404525	-5.670680
O	0.564995	3.026476	-2.352055	H	0.564223	2.249972	-6.643407
H	-0.151230	3.456778	-2.873282	O	-0.905645	3.431962	-6.646912
H	0.124354	2.680221	-1.541808	H	-1.059285	3.816304	-5.757068
O	-3.340067	2.052128	-3.956097	H	-1.649056	2.803445	-6.771034
H	-3.062971	1.357089	-3.314147	O	-2.822919	1.254535	-6.623038
H	-3.244497	1.662559	-4.855153	H	-2.114835	0.531829	-6.624820
O	-1.572980	4.081202	-3.905716	H	-3.501619	0.973052	-7.259201
H	-2.269378	3.359163	-3.864055	H-bq	-3.314024	0.894533	2.875325

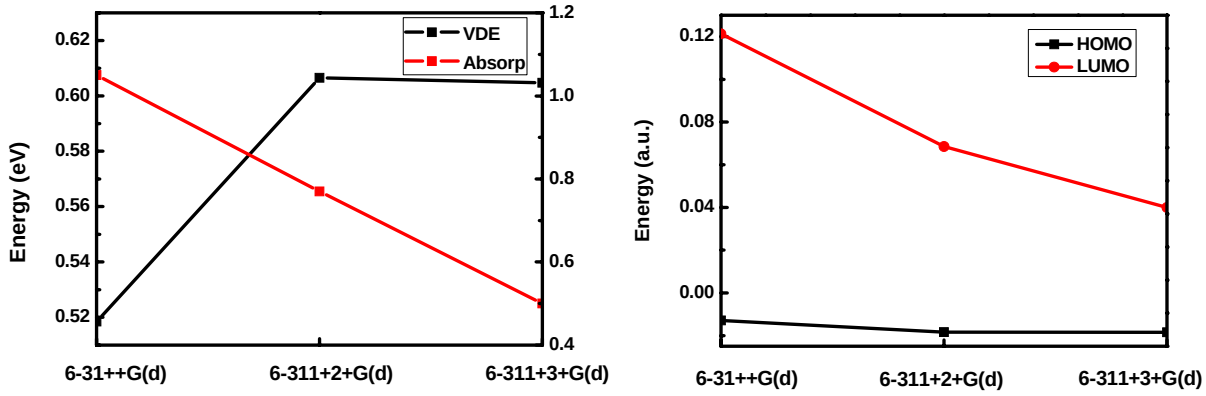


Figure S11. The calculated VDEs, the HOMO and LUMO energies of the $(H_2O)_{11}^-$ AA isomer, with respect to different atom-centered basis sets at the MP2 level. The UV absorption maxima shown in left are calculated at the TDDFT/B3LYP level.

Table S12. HOMO and LUMO distributions for the isomer Cub at the MP2 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.

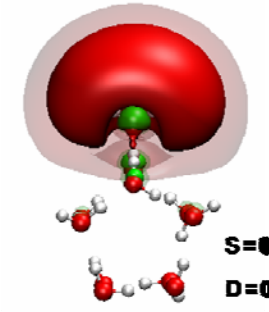
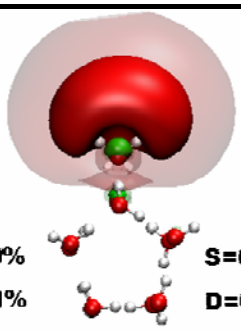
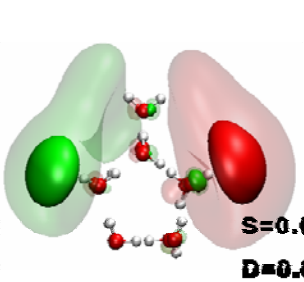
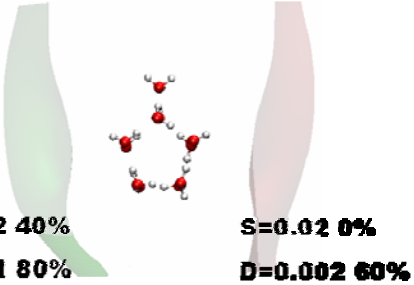
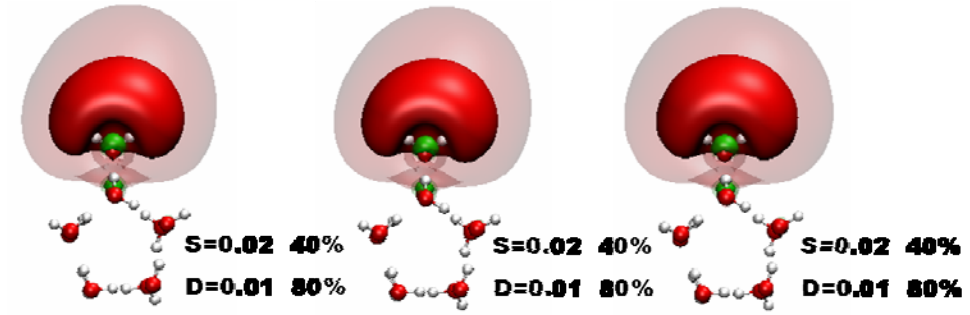
	6-31++G(d)	6-311+3+G(d)
HOMO	 S=0.02 60% D=0.01 90%	 S=0.02 35% D=0.01 80%
LUMO	 S=0.02 40% D=0.01 80%	 S=0.02 0% D=0.002 60%

Table S13. The HOMO and LUMO Distributions for the $(H_2O)_{20}^-$ $(5^{12})^-$A isomer, with respect to different atom-centered basis sets at the MP2 level. 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.

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