Supporting Information for

Systematic Parametrization of Divalent Metal Ions for the OPC3, OPC, TIP3P-FB, and TIP4P-FB Water Models

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Methods for Calculation for Ion-Water Clusters

The interaction energies of Mg^{2+}- H_2O and Ca^{2+}- H_2O in gas phase were evaluated for different ion parameter sets (*i.e.* the 12-6 HFE, 12-6 IOD, 12-6 CM and 12-6-4 parameter sets) along with different water models (*i.e.* the OPC3, OPC, TIP3P-FB, TIP4P-FB water models). The LEaP and ParmEd modules in the AmberTools19 software package[1] were used to generate the topologies. For each system, geometry optimization was performed through 2500 steps of minimization using the steepest descent algorithm followed by 2500 steps of minimization using the conjugate gradient algorithm. Afterwards, the optimized structure was used to calculate the ion-water interaction energy and ion-oxygen distance in the gas phase. No periodic boundary condition (PBC) was employed and the cut off value was set to 9999 Å. All these simulations were performed using the sander program in the Amber18 software package[1]. The vdW and electrostatic energies were extracted from the output file, and the sum of these two terms is the total interaction energy. We compared our results to the values obtained based on the Drude oscillator model, AMOEBA polarizable model, DFT (ωB97X-V/def2-QZVPPD) calculations reported in previous studies[2-3], as shown in Table 7 and Table S10.

The reaction energies of $[Zn(H_2O)_n]^{2+} + H_2O \rightarrow [Zn(H_2O)_{n+1}]^{2+}$, with n=0-5, were also calculated for different ion parameter sets (*i.e.* the 12-6 HFE, 12-6 IOD, 12-6 CM and 12-6-4 parameter sets) along with different water models (*i.e.* the OPC3, OPC, TIP3P-FB, TIP4P-FB water models). For each of the $[Zn(H_2O)_n]^{2+}$ complexes or H_2O molecule, its energy was computed based on the optimized geometry after 50000 steps of minimization (25000 steps using the steepest descent algorithm followed by 25000 steps using the conjugate gradient algorithm). Afterwards, the reaction energies were calculated. The calculated results are shown in Figure 5 and Table S11, along with the results from quantum mechanical (QM) calculations based on the MP4SDQ(FC)/HUZSP*//RHF/HUZSP* level of theory[4] for comparison.

Methods for Calculation for the Diffusivity Constants

The diffusion coefficient of Mg^{2+} was calculated for the 12-6 HFE, 12-6 IOD, 12-6 CM and 12-6-4 parameter sets with the OPC water model, using a protocol adapted from Panteva et al.[5] and Izadi et al.[6]. To simulate systems with different concentrations, a Mg^{2+} ion was solvated by four quasicubic boxes with box lengths of 40, 50, 58, and 62 Å, respectively. For each system, 10 individual simulations were performed as described below: (1) 5000 steps of minimization using the steepest descent algorithm followed by 5000 steps of minimization using the conjugate gradient algorithm; (2) 360 ps simulation using the NVT ensemble to gradually heat the system from 0 K to 300 K with a series of stages as described in the main text; (3) 2 ns equilibration using the NPT ensemble at 300 K and 1 atm; (4) 1 ns NVT simulation at 300 K to further equilibrate the system; (5) 2 ns simulations were performed which consisted of 80 successive cycles, with each cycle consisting of 5 ps of NPT equilibration followed by 20 ps NVE production with snapshots were saved every 0.2 ps. The cut off was set to 10.0 Å for all these simulations. The cpptraj program[7] in the AmberTools19 software package[8-9] was used to calculate the diffusion coefficient *D* of the Mg^{2+} ion for each of the 20 ps NVE production runs. Then the *D* values of the 80 NVT production runs were averaged to obtain the diffusion coefficient of the Mg^{2+} ion for the individual run. Afterwards, the diffusion coefficients of all 10 individual runs were averaged to get the size-dependent diffusion coefficient for a specific water box. To account for the intrinsic errors of different water models and make a more reasonable comparison with the experimental data, each of the size-dependent diffusion coefficients was then scaled by a factor of $2.3/D_w$, where 2.3 (unit is 10^{-5} cm^2/s) is the experimentally determined diffusion constant for water molecules while D_w is the averaged diffusion coefficient for water molecules inside that same water box. Finally, the diffusion coefficient of Mg^{2+} at infinite dilution D_o^{sim} was obtained using the equation below through extrapolation based on the four scaled size-dependent diffusion coefficients D_L:

$$D_o^{sim} = D_L + k\frac{1}{L}$$

Herein *k* is a constant which is related to viscosity, and *L* is length of the side of the water box. The error was calculated by multiplying the final result with the averaged percentage error of the four size-dependent diffusion coefficients, where the error of each was obtained as the standard deviation of the values obtained from the 10 individual runs. The final results are shown in Table 8.

For all of these minimizations and MD simulations, the periodic boundary conditions (PBCs) were used. The particle mesh Ewald (PME) method[10] was used to deal with the long-range electrostatic interactions. The nonbonded cutoff was set as 10 Å in these simulations. The "three-point" SHAKE algorithm[11] was used to constrain the geometries of the water molecules. The Langevin thermostat with a collision frequency of 2.0 ps^{-1} was used to control the temperature in all the MD simulations. The Berendsen barostat with a relaxation time of 1.0 ps was used to control the pressure in the NPT ensembles.

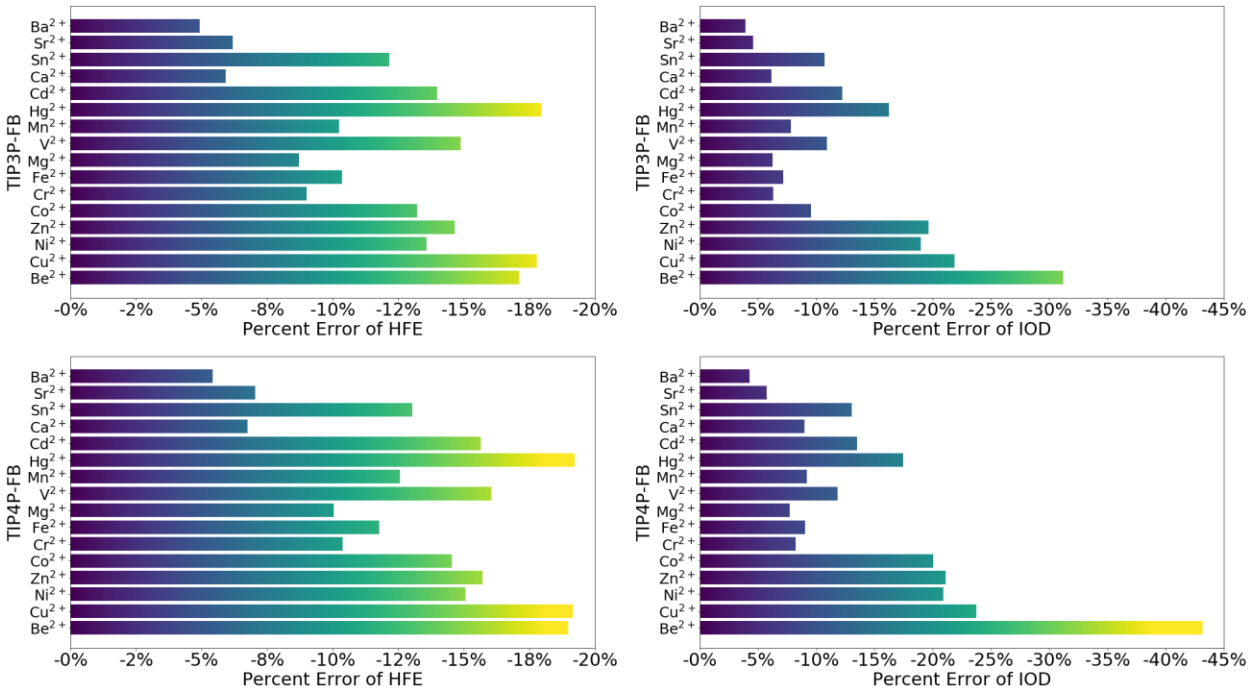

Figure S1. HFE and IOD percent errors for the 12-6 nonbonded model of metal ions in conjunction with the TIP3P-FB or TIP4P-FB water model. The HFE percent errors were for the 12-6 IOD parameter set that can reproduce the experimental IOD values (Tables 3 and S6). The IOD percent errors were for the 12-6 HFE parameter set that can reproduce the experimental HFE values (Tables 2 and S5).

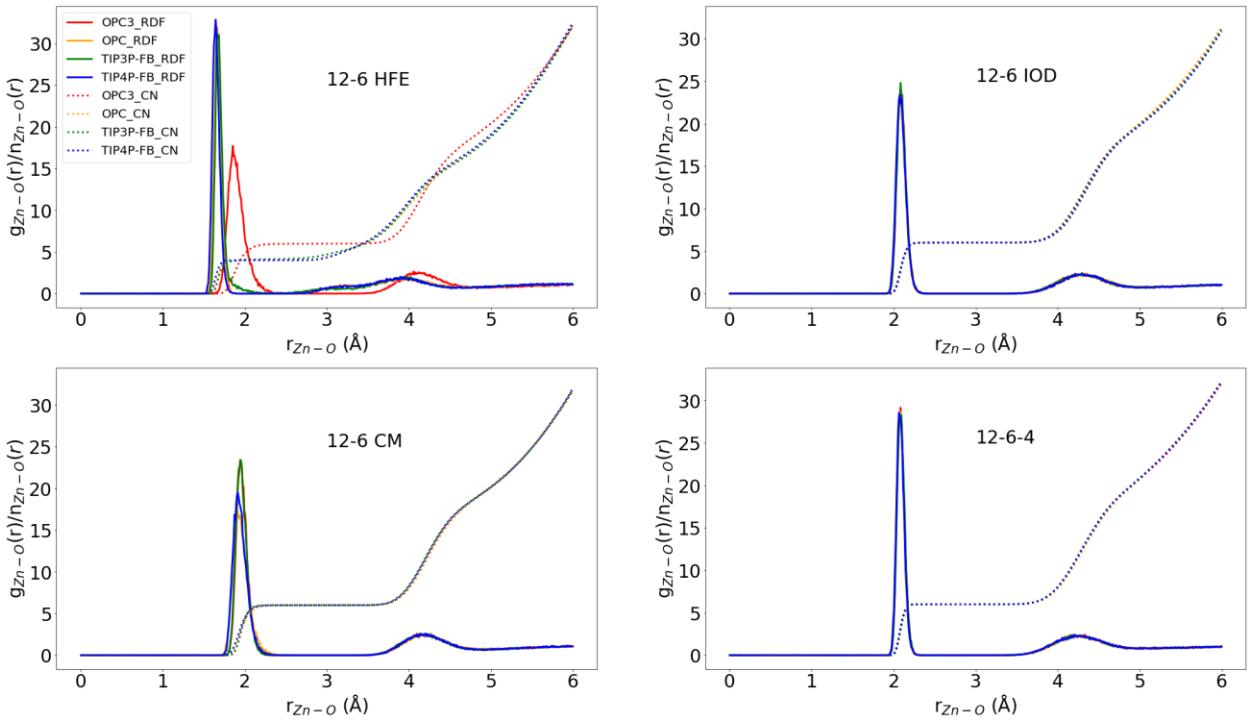

Figure S2. Radial distribution function (RDF) and cumulative coordination number between the Zn^{2+} ion and oxygen atoms of the water molecules, simulated by using different parameter sets along with different water models.

Table S1. Parameters for the Eight Different Water Models[a]

Water model	Q(O) or Q(M) (*e*)	Q(H) (*e*)	r(O-H) (Å)	H-O-H (°)	r(O-M) (Å)	R_{min}/2 for O (Å)	ε for O (kcal/mol)
TIP3P	-0.834	+0.417	0.9572	104.52	N/A	1.7683	0.1520
SPC/E	-0.8476	+0.4238	1.0	109.47	N/A	1.7767	0.1553
TIP4P	-1.04	+0.52	0.9572	104.52	0.15	1.7699	0.1550
TIP4P-Ew	-1.04844	+0.52422	0.9572	104.52	0.125	1.775931	0.16275
OPC3	-0.8952	+0.4476	0.9789	109.47	N/A	1.7814990	0.163406
OPC	-1.3582	+0.6791	0.8724	103.6	0.1594	1.777167268	0.2128008130
TIP3P-FB	-0.84844	+0.42422	1.0118	108.15	N/A	1.7835723	0.155866
TIP4P-FB	-1.05174	+0.52587	0.9572	104.52	0.10527	1.77660486	0.179082

[a]Herein M represents a dummy atom. For the 4-point water models, the oxygen atom has a charge of zero, while the dummy atom has a negative charge.

Table S2A. Convergence for Calculations of the HFE of Zn^{2+} Using the 12-6-4 Parameter Set and the OPC Water Model

Sampling in Each Window	Appearing of the VDW plus C_4 (kcal/mol)	Charge appearing (kcal/mol)	Charge disappearing (kcal/mol)	Disappearing of the VDW plus C_4 (kcal/mol)	Total HFE (kcal/mol)
100 ps w/ last 50 ps production	-47.73	-419.76	421.37	48.15	-468.50
200 ps w/ last 150 ps production	-47.96	-419.98	420.76	47.71	-468.21
300 ps w/ last 200 ps production	-47.99	-420.22	420.01	47.75	-467.99

Table S2B. Convergence for Calculations of the HFE of Zn^{2+} Using the CM Parameter Set and the OPC Water Model

Sampling in Each Window	VDW appearing (kcal/mol)	Charge appearing (kcal/mol)	Charge disappearing (kcal/mol)	VDW disappearing (kcal/mol)	Total HFE (kcal/mol)
100 ps w/ last 50 ps production	1.56	-444.71	444.99	-1.37	-443.38
200 ps w/ last 150 ps production	1.21	-445.36	444.28	-1.42	-443.51
300 ps w/ last 200 ps production	1.39	-443.98	444.93	-1.41	-443.06

Table S2C. Convergence for Calculations of the HFE and IOD of Zn^{2+} Using the 12-6-4 Parameter Set and the OPC Water Model by Varying the Size of the Charge Grid

Size of the charge grid along each dimension	HFE (kcal/mol)	Size of the charge grid along each dimension	IOD (Å)
36	-468.60	36	2.09
40	-468.03	40	2.09
48	-467.99	48	2.09
56	-467.69	56	2.09

Table S2D. Convergence for Calculations of the HFE and IOD of Zn^{2+} Using the CM Parameter Set and the OPC Water Model by Varying the Size of the Charge Grid

Size of the charge grid along each dimension	HFE (kcal/mol)	Size of the charge grid along each dimension	IOD (Å)
36	-443.33	36	1.93
40	-443.46	40	1.93
48	-443.06	48	1.93
56	-443.35	56	1.93

Table S3A. Calculated HFE Values from the Parameter Space Scans for the OPC3 Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C_4=0 kcal/mol*Å^4 (kcal/mol)	C_4=100 kcal/mol*Å^4 (kcal/mol)	C_4=200 kcal/mol*Å^4 (kcal/mol)	C_4=300 kcal/mol*Å^4 (kcal/mol)	C_4=400 kcal/mol*Å^4 (kcal/mol)
0.9	0.00000062	-588.3	N/A	-834.8	-937.7	-1039.0
1.0	0.00001422	-542.5	-642.3	-737.8	-833.4	-930.4
1.1	0.00016377	-510.6	-588.8	-673.9	-760.0	-847.7
1.2	0.00110429	-466.5	-524.5	-590.8	-664.4	-743.0
1.3	0.00490301	-439.7	-488.2	-541.0	-596.3	-656.0
1.4	0.01570749	-404.1	-445.3	-488.9	-533.4	-581.4
1.5	0.03899838	-369.8	-403.6	-438.1	-475.6	-513.3
1.6	0.07934493	-345.4	-375.0	-405.1	-436.9	-470.2
1.7	0.13818331	-325.2	-350.6	-376.7	-404.4	-433.4
1.8	0.21312875	-305.5	-328.5	-351.8	-377.4	-402.0
1.9	0.29896986	-288.9	-309.7	-331.0	-352.6	-375.4
2.0	0.38943250	-273.7	-292.7	-311.7	-331.7	-352.7
2.1	0.47874242	-260.4	-277.7	-295.5	-313.7	-332.5
2.2	0.56252208	-248.6	-264.9	-281.7	-298.0	-315.9
2.3	0.63803333	-237.3	-253.0	-268.6	-284.4	-300.2

[a]Herein "N/A" means the job failed along the simulation process. This point was not used in the curve fitting.

Table S3B. Calculated HFE Values from the Parameter Space Scans for the OPC Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C_4=0 kcal/mol*Å^4 (kcal/mol)	C_4=100 kcal/mol*Å^4 (kcal/mol)	C_4=200 kcal/mol*Å^4 (kcal/mol)	C_4=300 kcal/mol*Å^4 (kcal/mol)	C_4=400 kcal/mol*Å^4 (kcal/mol)
0.9	0.00000062	-556.0	-680.0	-786.5	N/A	N/A
1.0	0.00001422	-514.6	-609.1	-703.1	-795.5	-887.9
1.1	0.00016377	-485.7	-557.8	-639.0	-720.4	-803.5
1.2	0.00110429	-446.9	-501.6	-564.6	-632.7	-708.2
1.3	0.00490301	-422.4	-468.4	-518.7	-569.0	-623.5
1.4	0.01570749	-389.4	-429.0	-469.5	-511.9	-557.4
1.5	0.03899838	-357.4	-389.4	-422.7	-458.1	-494.8
1.6	0.07934493	-336.3	-364.1	-393.5	-423.5	-455.2
1.7	0.13818331	-315.4	-340.4	-366.3	-393.1	-421.7
1.8	0.21312875	-297.6	-322.0	-344.2	-367.8	-392.4
1.9	0.29896986	-282.8	-302.9	-324.4	-345.8	-365.2
2.0	0.38943250	-267.7	-288.5	-306.8	-325.7	-346.2
2.1	0.47874242	-255.0	-269.7	-291.4	-309.4	-325.6
2.2	0.56252208	-243.3	-261.8	-277.5	-294.0	-309.7
2.3	0.63803333	-233.0	-249.3	-265.4	-280.8	-297.3

[a]Herein "N/A" means the job failed along the simulation process. These points were not used in the curve fittings.

Table S3C. Calculated HFE Values from the Parameter Space Scans for the TIP3P-FB Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C_4=0 kcal/mol*Å^4 (kcal/mol)	C_4=100 kcal/mol*Å^4 (kcal/mol)	C_4=200 kcal/mol*Å^4 (kcal/mol)	C_4=300 kcal/mol*Å^4 (kcal/mol)	C_4=400 kcal/mol*Å^4 (kcal/mol)
0.9	0.00000062	-578.8	-708.3	-823.1	-924.8	N/A
1.0	0.00001422	-533.9	-632.5	-729.2	-824.3	-920.8
1.1	0.00016377	-503.0	-580.8	-665.8	-752.3	-840.1
1.2	0.00110429	-460.0	-518.6	-584.4	-659.0	-736.5
1.3	0.00490301	-434.2	-483.4	-535.5	-591.5	-651.3
1.4	0.01570749	-399.6	-439.9	-483.4	-528.4	-575.6
1.5	0.03899838	-365.6	-399.4	-434.5	-470.6	-509.0
1.6	0.07934493	-342.0	-371.1	-402.0	-433.6	-467.5
1.7	0.13818331	-321.2	-346.9	-373.0	-401.2	-430.2
1.8	0.21312875	-302.7	-325.9	-348.6	-373.6	-399.7
1.9	0.29896986	-286.2	-307.4	-328.1	-350.4	-372.9
2.0	0.38943250	-271.2	-290.4	-309.4	-329.1	-349.9
2.1	0.47874242	-258.7	-275.5	-293.8	-311.9	-330.4
2.2	0.56252208	-246.5	-263.3	-279.3	-296.4	-313.7
2.3	0.63803333	-236.1	-251.1	-266.8	-282.0	-298.7

[a]Herein "N/A" means the job failed along the simulation process. This point was not used in the curve fitting.

Table S3D. Calculated HFE Values from the Parameter Space Scans for the TIP4P-FB Water Model[a]

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C_4=0 kcal/mol*Å^4 (kcal/mol)	C_4=100 kcal/mol*Å^4 (kcal/mol)	C_4=200 kcal/mol*Å^4 (kcal/mol)	C_4=300 kcal/mol*Å^4 (kcal/mol)	C_4=400 kcal/mol*Å^4 (kcal/mol)
0.9	0.00000062	-552.2	-678.5	N/A	N/A	N/A
1.0	0.00001422	-512.0	-607.8	-703.1	-794.5	-890.7
1.1	0.00016377	-482.9	-558.9	-641.9	-726.3	-812.6
1.2	0.00110429	-445.8	-501.2	-564.8	-636.2	-713.5
1.3	0.00490301	-420.8	-469.4	-519.7	-573.3	-630.3
1.4	0.01570749	-388.7	-428.1	-470.1	-514.4	-560.5
1.5	0.03899838	-357.0	-388.1	-422.9	-459.1	-495.2
1.6	0.07934493	-334.9	-363.3	-392.6	-424.5	-457.6
1.7	0.13818331	-315.5	-340.3	-366.2	-394.0	-421.4
1.8	0.21312875	-297.9	-320.6	-344.0	-367.7	-392.7
1.9	0.29896986	-282.1	-302.6	-323.1	-345.7	-367.5
2.0	0.38943250	-267.7	-286.9	-306.2	-325.2	-345.6
2.1	0.47874242	-255.2	-272.6	-290.1	-308.7	-327.4
2.2	0.56252208	-243.8	-260.1	-276.2	-293.7	-311.1
2.3	0.63803333	-234.4	-249.2	-264.7	-280.3	-295.3

[a]Herein "N/A" means the job failed along the simulation process. These points were not used in the curve fittings.

Table S3E. Calculated HFE Values from the Parameter Scans for the TIP3P, SPC/E, TIP4P, and TIP4P-Ew Water Models

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	TIP3P C_4=0 kcal/mol*Å^4 (kcal/mol)	SPC/E C_4=0 kcal/mol*Å^4 (kcal/mol)	TIP4P C_4=0 kcal/mol*Å^4 (kcal/mol)	TIP4P-Ew C_4=0 kcal/mol*Å^4 (kcal/mol)
0.9	0.00000062	-575.7	-578.4	-520.5	-539.5
1.0	0.00001422	-530.2	-533.4	-485.0	-500.9
1.1	0.00016377	-499.8	-502.6	-458.4	-472.8
1.2	0.00110429	-460.8	-460.7	-425.9	-439.3
1.3	0.00490301	-432.5	-433.8	-401.2	-413.1
1.4	0.01570749	-397.9	-398.6	-370.2	-380.8
1.5	0.03899838	-366.4	-364.6	-343.1	-351.7
1.6	0.07934493	-344.2	-342.8	-324.1	-330.7
1.7	0.13818331	-324.2	-321.9	-305.2	-311.0
1.8	0.21312875	-306.1	-303.4	-289.9	-294.7
1.9	0.29896986	-290.3	-286.6	-275.2	-279.2
2.0	0.38943250	-275.9	-271.9	-261.9	-265.1
2.1	0.47874242	-263.1	-259.3	-249.9	-253.6
2.2	0.56252208	-251.2	-247.6	-239.2	-243.0
2.3	0.63803333	-241.0	-237.0	-230.8	-233.1

Table S4A. Calculated IOD and CN Values from the Parameter Space Scans for the OPC3 Water Model

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=100 kcal/mol*Å^4		C4=200 kcal/mol*Å^4		C4=300 kcal/mol*Å^4		C4=400 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.14	2.0	N/A	N/A	1.03	2.0	0.99	2.0	0.97	2.0
1.0	0.00001422	1.40	3.0	1.30	2.0	1.19	2.0	1.14	2.0	1.11	2.0
1.1	0.00016377	1.59	4.0	1.54	4.0	1.51	4.0	1.48	4.0	1.45	4.0
1.2	0.00110429	1.87	6.0	1.68	4.4	1.64	4.0	1.61	4.0	1.58	4.0
1.3	0.00490301	1.98	6.0	1.94	6.0	1.91	6.0	1.88	6.0	1.86	6.0
1.4	0.01570749	2.09	6.0	2.06	6.0	2.03	6.0	2.01	6.0	1.98	6.0
1.5	0.03899838	2.25	6.4	2.21	6.3	2.19	6.5	2.15	6.1	2.12	6.1
1.6	0.07934493	2.44	7.8	2.42	7.9	2.39	8.0	2.37	8.0	2.35	8.0
1.7	0.13818331	2.56	8.0	2.54	8.0	2.51	8.1	2.49	8.2	2.47	8.2
1.8	0.21312875	2.69	8.5	2.67	8.7	2.65	8.9	2.63	9.0	2.62	9.0
1.9	0.29896986	2.81	8.9	2.79	9.0	2.77	9.1	2.75	9.1	2.73	9.2
2.0	0.38943250	2.92	9.2	2.91	9.4	2.89	9.5	2.87	9.7	2.86	9.8
2.1	0.47874242	3.04	9.6	3.02	9.8	3.00	10.0	2.99	10.1	2.97	10.2
2.2	0.56252208	3.14	10.0	3.13	10.3	3.11	10.6	3.10	10.7	3.09	11.0
2.3	0.63803333	3.25	10.6	3.23	10.7	3.22	10.9	3.21	11.3	3.19	11.3

Table S4B. Calculated IOD and CN Values from the Parameter Space Scans for the OPC Water Model

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=100 kcal/mol*Å^4		C4=200 kcal/mol*Å^4		C4=300 kcal/mol*Å^4		C4=400 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.16	2.0	1.10	2.0	1.05	2.0	N/A	N/A	N/A	N/A
1.0	0.00001422	1.43	2.0	1.27	2.0	1.20	2.0	1.16	2.0	1.13	2.0
1.1	0.00016377	1.62	4.0	1.58	4.0	1.54	4.0	1.51	4.0	1.48	4.0
1.2	0.00110429	1.90	6.0	1.70	4.1	1.67	4.0	1.64	4.0	1.61	4.0
1.3	0.00490301	2.01	6.0	1.98	6.0	1.94	6.0	1.92	6.0	1.89	6.0
1.4	0.01570749	2.12	6.0	2.09	6.0	2.06	6.0	2.04	6.0	2.01	6.0
1.5	0.03899838	2.28	6.5	2.25	6.5	2.22	6.4	2.19	6.7	2.16	6.7
1.6	0.07934493	2.48	7.9	2.45	6.5	2.43	8.0	2.41	8.0	2.38	8.0
1.7	0.13818331	2.60	8.2	2.57	8.3	2.55	8.3	2.53	8.4	2.52	8.6
1.8	0.21312875	2.73	8.9	2.71	6.5	2.69	9.0	2.67	9.0	2.65	9.0
1.9	0.29896986	2.85	9.1	2.82	9.2	2.81	9.2	2.79	9.3	2.77	9.6
2.0	0.38943250	2.96	9.5	2.95	9.7	2.93	9.9	2.91	10.0	2.90	10.0
2.1	0.47874242	3.08	10.0	3.06	10.2	3.05	10.3	3.03	10.6	3.02	11.0
2.2	0.56252208	3.19	10.5	3.17	10.7	3.16	11.0	3.15	11.3	3.14	11.5
2.3	0.63803333	3.30	11.0	3.28	11.1	3.27	11.5	3.25	11.8	3.24	11.8

Table S4C. Calculated IOD and CN Values from the Parameter Space Scans for the TIP3P-FB Water Model

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=100 kcal/mol*Å^4		C4=200 kcal/mol*Å^4		C4=300 kcal/mol*Å^4		C4=400 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.14	2.0	1.07	2.0	1.02	2.0	0.99	2.0	N/A	N/A
1.0	0.00001422	1.41	3.0	1.32	3.0	1.18	2.0	1.14	2.0	1.11	2.0
1.1	0.00016377	1.59	4.0	1.54	4.0	1.51	4.0	1.48	4.0	1.45	4.0
1.2	0.00110429	1.87	6.0	1.68	4.9	1.64	4.0	1.61	4.0	1.58	4.0
1.3	0.00490301	1.98	6.0	1.94	6.0	1.91	6.0	1.88	6.0	1.86	6.0
1.4	0.01570749	2.09	6.0	2.06	6.0	2.03	6.0	2.00	6.0	1.98	6.0
1.5	0.03899838	2.25	6.4	2.22	6.4	2.20	6.5	2.16	6.3	2.14	6.4
1.6	0.07934493	2.44	7.8	2.42	7.9	2.39	8.0	2.37	8.0	2.35	8.0
1.7	0.13818331	2.56	8.0	2.53	8.1	2.51	8.1	2.49	8.2	2.47	8.3
1.8	0.21312875	2.69	8.6	2.67	8.7	2.65	8.9	2.63	9.0	2.61	9.0
1.9	0.29896986	2.81	8.9	2.79	9.0	2.77	9.1	2.75	9.1	2.73	9.2
2.0	0.38943250	2.92	9.2	2.91	9.3	2.89	9.5	2.87	9.7	2.86	9.9
2.1	0.47874242	3.03	9.6	3.02	9.8	3.00	10.0	2.99	10.1	2.97	10.3
2.2	0.56252208	3.14	10.0	3.13	10.2	3.12	10.4	3.10	9.4	3.09	11.1
2.3	0.63803333	3.25	10.6	3.24	10.9	3.22	11.0	3.21	11.3	3.20	11.5

Table S4D. Calculated IOD and CN Values from the Parameter Space Scans for the TIP4P-FB Water Model

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	C4=0 kcal/mol*Å^4		C4=100 kcal/mol*Å^4		C4=200 kcal/mol*Å^4		C4=300 kcal/mol*Å^4		C4=400 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.15	2.0	1.08	2.0	N/A	N/A	N/A	N/A	N/A	N/A
1.0	0.00001422	1.42	3.0	1.29	3.0	1.19	2.0	1.15	2.0	1.12	2.0
1.1	0.00016377	1.60	4.0	1.56	4.0	1.52	4.0	1.49	4.0	1.47	4.0
1.2	0.00110429	1.89	6.0	1.70	4.8	1.65	4.0	1.62	4.0	1.59	4.0
1.3	0.00490301	1.99	6.0	1.96	6.0	1.93	6.0	1.90	6.0	1.87	6.0
1.4	0.01570749	2.11	6.0	2.08	6.0	2.04	6.0	2.02	6.0	1.99	6.0
1.5	0.03899838	2.28	6.8	2.25	6.7	2.23	6.8	2.19	6.7	2.17	6.7
1.6	0.07934493	2.46	7.9	2.43	8.0	2.41	8.0	2.39	8.0	2.36	8.0
1.7	0.13818331	2.58	8.1	2.55	8.2	2.53	8.3	2.52	8.5	2.50	8.7
1.8	0.21312875	2.71	8.9	2.69	8.9	2.67	9.0	2.65	9.0	2.63	9.0
1.9	0.29896986	2.83	9.0	2.81	9.2	2.79	9.2	2.77	9.3	2.75	9.5
2.0	0.38943250	2.95	9.5	2.93	9.7	2.91	9.8	2.89	9.9	2.88	10.0
2.1	0.47874242	3.06	9.9	3.04	10.1	3.02	10.2	3.01	10.4	3.00	10.7
2.2	0.56252208	3.17	10.4	3.15	10.6	3.14	10.9	3.13	11.2	3.12	11.4
2.3	0.63803333	3.28	11.0	3.26	11.1	3.25	11.4	3.24	11.5	3.22	11.6

Table S4E. Calculated IOD and CN Values from the Parameter Scans for the TIP3P, SPC/E, TIP4P, and TIP4P-Ew Water Models

$R_{min,M}/2$ (Å)	ε_M (kcal/mol)	TIP3P C4=0 kcal/mol*Å^4		SPC/E C4=0 kcal/mol*Å^4		TIP4P C4=0 kcal/mol*Å^4		TIP4P-Ew C4=0 kcal/mol*Å^4	
		IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN	IOD (Å)	CN
0.9	0.00000062	1.13	2.0	1.13	2.0	1.15	2.0	1.15	2.0
1.0	0.00001422	1.40	3.0	1.40	3.0	1.42	3.0	1.42	3.0
1.1	0.00016377	1.58	4.0	1.58	4.0	1.60	4.0	1.60	4.0
1.2	0.00110429	1.86	6.0	1.87	6.0	1.88	6.0	1.89	6.0
1.3	0.00490301	1.96	6.0	1.97	6.0	1.98	6.0	1.99	6.0
1.4	0.01570749	2.08	6.0	2.09	6.0	2.10	6.0	2.10	6.0
1.5	0.03899838	2.28	7.1	2.26	6.7	2.31	7.4	2.30	7.0
1.6	0.07934493	2.44	8.0	2.44	7.9	2.46	8.0	2.46	8.0
1.7	0.13818331	2.56	8.3	2.56	8.0	2.59	8.7	2.58	8.3
1.8	0.21312875	2.69	8.9	2.69	8.7	2.71	9.0	2.71	8.9
1.9	0.29896986	2.80	9.1	2.80	9.0	2.83	9.3	2.82	9.1
2.0	0.38943250	2.92	9.6	2.92	9.3	2.95	9.9	2.94	9.6
2.1	0.47874242	3.03	10.0	3.03	9.8	3.06	10.2	3.06	10.0
2.2	0.56252208	3.14	10.4	3.14	10.0	3.17	10.9	3.16	10.5
2.3	0.63803333	3.24	10.9	3.25	10.6	3.28	11.4	3.27	11.0

Table S5. Calculated HFE, IOD, and CN Values for the HFE Parameter Set for the Four Water Models (Parameters in Table 2)

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Be^{2+}	-572.3	1.18	2.0	-571.7	0.98	1.0	-573.1	1.15	2.0	-572.2	0.95	1.0
Cu^{2+}	-480.2	1.66	4.0	-481.1	1.63	4.0	-479.8	1.65	4.0	-480.4	1.61	4.0
Ni^{2+}	-473.9	1.68	4.0	-473.8	1.65	4.0	-472.2	1.67	4.0	-473.3	1.63	4.0
Pt^{2+}	-468.9	1.86	5.9	-469.5	1.67	4.0	-468.8	1.68	4.0	-468.6	1.65	4.0
Zn^{2+}	-466.6	1.87	6.0	-466.8	1.67	4.0	-467.0	1.68	4.1	-466.7	1.65	4.0
Co^{2+}	-457.3	1.91	6.0	-457.7	1.70	4.0	-456.7	1.90	6.0	-457.6	1.68	4.0
Pd^{2+}	-456.5	1.92	6.0	-456.5	1.71	4.0	-456.7	1.90	6.0	-456.0	1.68	4.0
Ag^{2+}	-445.1	1.96	6.0	-444.9	1.91	6.0	-445.9	1.94	6.0	-445.8	1.89	6.0
Cr^{2+}	-442.4	1.97	6.0	-443.1	1.93	6.0	-441.2	1.95	6.0	-442.2	1.91	6.0
Fe^{2+}	-439.7	1.98	6.0	-440.2	1.94	6.0	-439.7	1.96	6.0	-439.7	1.92	6.0
Mg^{2+}	-437.8	1.98	6.0	-436.9	1.95	6.0	-437.9	1.96	6.0	-437.7	1.93	6.0
V^{2+}	-435.9	1.99	6.0	-437.1	1.95	6.0	-437.2	1.97	6.0	-436.2	1.95	6.0
Mn^{2+}	-421.4	2.04	6.0	-420.4	2.01	6.0	-420.6	2.02	6.0	-420.8	1.99	6.0
Hg^{2+}	-420.7	2.04	6.0	-420.4	2.01	6.0	-420.6	2.02	6.0	-420.8	1.99	6.0
Cd^{2+}	-419.5	2.04	6.0	-419.0	2.02	6.0	-420.1	2.02	6.0	-419.8	1.99	6.0
Yb^{2+}	-361.2	2.33	7.0	-360.9	2.25	6.3	-360.7	2.31	6.9	-360.5	2.23	6.2
Ca^{2+}	-358.9	2.34	7.1	-359.4	2.26	6.4	-359.4	2.31	6.9	-359.8	2.24	6.4
Sn^{2+}	-355.2	2.36	7.2	-356.5	2.31	6.8	-355.4	2.34	7.1	-357.0	2.28	6.7
Pb^{2+}	-340.3	2.47	7.9	-339.8	2.44	7.8	-340.1	2.45	7.8	-340.1	2.42	7.8
Eu^{2+}	-331.0	2.53	8.0	-331.2	2.51	8.0	-331.3	2.51	8.0	-330.4	2.49	8.0
Sr^{2+}	-329.4	2.54	8.0	-329.6	2.51	8.0	-330.3	2.52	8.0	-329.9	2.49	8.0
Sm^{2+}	-327.8	2.54	8.0	-328.9	2.52	8.0	-328.9	2.52	8.0	-328.8	2.50	8.0
Ba^{2+}	-298.9	2.74	8.8	-298.4	2.73	8.9	-299.3	2.72	8.7	-298.4	2.71	8.8
Ra^{2+}	-298.5	2.74	8.8	-298.4	2.73	8.8	-299.3	2.72	8.7	-298.3	2.70	8.8

Table S6. Calculated HFE, IOD, and CN Values for the IOD Parameter Set for the Four Water Models (Parameters in Table 3)

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Be^{2+}	-482.1	1.66	4.0	-472.2	1.66	4.0	-474.4	1.66	4.0	-463.8	1.66	4.0
Cu^{2+}	-400.1	2.11	6.0	-392.7	2.11	6.0	-395.0	2.11	6.0	-388.3	2.11	6.0
Ni^{2+}	-413.6	2.06	6.0	-407.6	2.06	6.0	-409.0	2.06	6.0	-401.9	2.06	6.0
Zn^{2+}	-404.0	2.09	6.0	-399.6	2.09	6.0	-398.8	2.09	6.0	-393.9	2.09	6.0
Co^{2+}	-401.6	2.10	6.0	-395.9	2.10	6.0	-397.2	2.10	6.0	-391.1	2.10	6.0
Cr^{2+}	-407.4	2.08	6.0	-401.8	2.08	6.0	-402.4	2.08	6.0	-396.3	2.08	6.0
Fe^{2+}	-399.5	2.11	6.0	-392.9	2.11	6.0	-394.3	2.11	6.0	-388.0	2.11	6.0
Mg^{2+}	-404.2	2.09	6.0	-398.2	2.09	6.0	-399.3	2.09	6.0	-393.5	2.09	6.0
V^{2+}	-376.4	2.20	6.0	-371.3	2.20	6.0	-371.3	2.20	6.0	-366.2	2.20	6.0
Mn^{2+}	-382.1	2.18	6.0	-375.0	2.18	6.0	-377.6	2.18	6.0	-367.9	2.19	6.0
Hg^{2+}	-349.6	2.41	7.6	-342.9	2.42	7.7	-345.1	2.41	7.6	-339.8	2.42	7.8
Cd^{2+}	-363.0	2.31	6.9	-355.9	2.31	6.8	-360.9	2.31	6.9	-353.9	2.31	7.0
Ca^{2+}	-341.2	2.46	7.9	-337.9	2.46	7.9	-338.4	2.46	7.9	-335.4	2.46	7.9
Sn^{2+}	-315.6	2.62	8.1	-313.0	2.62	8.3	-312.8	2.62	8.2	-309.7	2.62	8.4
Sr^{2+}	-313.2	2.64	8.2	-310.2	2.64	8.4	-309.4	2.64	8.3	-306.6	2.64	8.4
Ba^{2+}	-285.8	2.83	9.0	-284.8	2.83	9.1	-284.1	2.83	9.0	-282.6	2.83	9.1

Table S7. Calculated HFE, IOD, and CN Values for the CM Parameter Set for the Four Water Models (Parameters in Table 4)

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Be^{2+}	-551.8	1.25	1.9	-547.7	1.18	2.0	-546.9	1.23	2.0	-542.5	1.18	2.0
Cu^{2+}	-459.6	1.91	6.0	-454.9	1.71	4.0	-455.9	1.90	6.0	-448.3	1.71	4.6
Ni^{2+}	-454.0	1.93	6.0	-448.0	1.90	5.9	-448.7	1.93	6.0	-443.8	1.90	6.0
Pt^{2+}	-450.8	1.95	6.0	-444.8	1.93	6.0	-442.9	1.95	6.0	-438.1	1.99	6.0
Zn^{2+}	-446.9	1.96	6.0	-443.1	1.93	6.0	-442.8	1.95	6.0	-437.9	1.93	6.0
Co^{2+}	-437.8	1.98	6.0	-434.5	1.97	6.0	-432.8	1.98	6.0	-428.8	1.97	6.0
Pd^{2+}	-436.6	1.99	6.0	-431.7	1.98	6.0	-431.3	1.99	6.0	-425.9	1.97	6.0
Ag^{2+}	-426.3	2.02	6.0	-421.0	2.01	6.0	-421.6	2.02	6.0	-415.9	2.01	6.0
Cr^{2+}	-422.9	2.03	6.0	-417.1	2.03	6.0	-417.5	2.03	6.0	-412.1	2.02	6.0
Fe^{2+}	-420.1	2.04	6.0	-414.7	2.03	6.0	-414.9	2.04	6.0	-410.1	2.03	6.0
Mg^{2+}	-417.8	2.05	6.0	-412.4	2.04	6.0	-412.5	2.05	6.0	-407.6	2.04	6.0
V^{2+}	-416.1	2.05	6.0	-411.7	2.04	6.0	-411.3	2.05	6.0	-406.2	2.04	6.0
Mn^{2+}	-400.6	2.11	6.0	-396.1	2.10	6.0	-395.5	2.11	6.0	-390.5	2.10	6.0
Hg^{2+}	-400.0	2.11	6.0	-396.7	2.10	6.0	-395.4	2.11	6.0	-389.7	2.10	6.0
Cd^{2+}	-399.5	2.11	6.0	-393.5	2.11	6.0	-393.8	2.11	6.0	-388.8	2.11	6.0
Yb^{2+}	-340.7	2.47	7.9	-336.5	2.48	7.9	-335.4	2.48	7.9	-330.2	2.49	8.0
Ca^{2+}	-339.6	2.48	7.9	-334.8	2.49	7.9	-334.3	2.49	7.9	-330.2	2.49	8.0
Sn^{2+}	-335.6	2.49	8.0	-331.3	2.51	8.0	-331.8	2.51	8.0	-326.2	2.51	8.0
Pb^{2+}	-320.1	2.59	8.1	-315.3	2.60	8.2	-316.0	2.60	8.1	-310.0	2.61	8.3
Eu^{2+}	-310.6	2.65	8.4	-306.6	2.67	8.6	-306.5	2.67	8.4	-301.1	2.69	8.7
Sr^{2+}	-309.5	2.66	8.4	-306.5	2.69	8.7	-304.7	2.68	8.5	-299.0	2.70	8.8
Sm^{2+}	-309.0	2.67	8.4	-304.1	2.69	8.7	-303.1	2.68	8.5	-297.9	2.71	8.8
Ba^{2+}	-278.3	2.88	9.1	-275.2	2.91	9.4	-274.2	2.90	9.2	-269.8	2.94	9.4
Ra^{2+}	-279.0	2.88	9.1	-274.5	2.91	9.3	-273.9	2.90	9.1	-269.5	2.93	9.4

Table S8. Calculated HFE, IOD, and CN Values for the 12-6-4 Parameter Set for the Four Water Models (Parameters in Table 5)

	OPC3			OPC			TIP3P-FB			TIP4P-FB		
	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN	HFE (kcal/mol)	IOD (Å)	CN
Be^{2+}	-571.7	1.66	4.5	-572.8	1.66	4.0	-572.4	1.66	4.5	-572.8	1.67	4.9
Cu^{2+}	-480.7	2.11	6.0	-480.6	2.10	6.0	-480.3	2.10	6.0	-479.6	2.11	6.0
Ni^{2+}	-473.6	2.07	6.0	-473.8	2.06	6.0	-473.8	2.07	5.8	-473.1	2.05	6.0
Zn^{2+}	-467.3	2.09	6.0	-468.0	2.09	6.0	-466.9	2.09	6.0	-468.1	2.08	6.0
Co^{2+}	-458.7	2.09	6.0	-458.1	2.10	6.0	-457.3	2.09	6.0	-456.6	2.09	6.0
Cr^{2+}	-442.7	2.08	6.0	-441.7	2.08	6.0	-442.0	2.09	6.0	-441.8	2.09	6.0
Fe^{2+}	-439.6	2.11	6.0	-439.8	2.11	6.0	-439.2	2.12	6.0	-440.1	2.12	6.0
Mg^{2+}	-438.0	2.10	6.0	-437.6	2.09	6.0	-437.3	2.10	6.0	-438.0	2.08	6.0
V^{2+}	-437.1	2.20	6.5	-436.1	2.22	6.5	-437.2	2.22	6.8	-436.5	2.20	6.0
Mn^{2+}	-420.5	2.19	6.2	-420.3	2.19	6.0	-420.0	2.18	6.1	-420.4	2.18	6.2
Hg^{2+}	-421.1	2.41	8.0	-419.7	2.41	8.0	-420.9	2.41	8.0	-421.7	2.42	8.0
Cd^{2+}	-420.4	2.31	7.4	-420.0	2.30	7.3	-419.2	2.30	7.4	-419.0	2.31	7.6
Ca^{2+}	-359.5	2.46	8.0	-360.1	2.46	8.0	-359.4	2.47	8.0	-360.1	2.46	8.0
Sn^{2+}	-355.6	2.62	8.7	-356.1	2.62	8.8	-356.6	2.62	8.8	-355.9	2.62	8.9
Sr^{2+}	-329.8	2.64	8.5	-330.2	2.63	8.6	-329.6	2.63	8.5	-329.7	2.64	8.8
Ba^{2+}	-298.9	2.84	9.1	-299.4	2.83	9.1	-298.6	2.82	9.1	-298.3	2.83	9.2

Table S9. vdW Radii ($R_{min}/2$ values) of Different Parameter Sets and Their Statistical Analysis against Quantum Scaling Principle Calculated Values (See Figure 4 in the Main Text)

	Previous			OPC3			OPC		
	Åqvist[a]	Babu and Lim Set 1[b]	Babu and Lim Set 2[c]	HFE	IOD	12-6-4	HFE	IOD	12-6-4
Mg^{2+}	0.787	1.183	1.364	1.306	1.400	1.433	1.239	1.373	1.405
Ca^{2+}	1.326	1.831	1.936	1.541	1.617	1.632	1.493	1.590	1.602
Sr^{2+}	1.742	1.968	2.092	1.677	1.762	1.777	1.631	1.731	1.738
Ba^{2+}	2.124	2.062	2.245	1.840	1.918	1.936	1.797	1.883	1.898
Average Error (Å)	-0.027	0.239	0.388	0.069	0.152	0.173	0.018	0.122	0.139
Standard Deviation (Å)	0.270	0.141	0.118	0.034	0.040	0.047	0.024	0.042	0.050
AUE (Å)	0.246	0.239	0.388	0.069	0.152	0.173	0.021	0.122	0.139

	TIP3P-FB			TIP4P-FB		
	HFE	IOD	12-6-4	HFE	IOD	12-6-4
Mg^{2+}	1.288	1.400	1.433	1.238	1.383	1.409
Ca^{2+}	1.525	1.617	1.636	1.488	1.600	1.625
Sr^{2+}	1.659	1.762	1.769	1.626	1.746	1.755
Ba^{2+}	1.824	1.918	1.922	1.795	1.900	1.917
Average Error (Å)	0.052	0.152	0.168	0.015	0.136	0.155
Standard Deviation (Å)	0.033	0.040	0.051	0.025	0.040	0.044
AUE (Å)	0.052	0.152	0.168	0.018	0.136	0.155

[a]From Ref.[12].
[b]From Ref.[13] by reproducing the relative HFEs towards Zn^{2+}.
[c]From Ref.[13] by reproducing the relative HFEs towards Cd^{2+}.

Table S10. Benchmark Calculations for the Ion-Water Dimer Systems Containing Mg^{2+} or Ca^{2+} Using the OPC, TIP3P-FB, and TIP4P-FB Water Models

Ion	Model	Water Model	Interaction Energy (kcal/mol)	IOD (Å)
Mg^{2+}-H_2O dimer				
Mg^{2+}	12-6 HFE	OPC	-102.92	1.72
Mg^{2+}	12-6 IOD	OPC	-80.43	1.97
Mg^{2+}	12-6 CM	OPC	-86.58	1.89
Mg^{2+}	12-6-4	OPC	-84.50	1.99
Mg^{2+}	12-6 HFE	TIP3P-FB	-84.05	1.81
Mg^{2+}	12-6 IOD	TIP3P-FB	-69.44	2.00
Mg^{2+}	12-6 CM	TIP3P-FB	-73.69	1.94
Mg^{2+}	12-6-4	TIP3P-FB	-73.55	2.02
Mg^{2+}	12-6 HFE	TIP4P-FB	-92.69	1.72
Mg^{2+}	12-6 IOD	TIP4P-FB	-71.55	1.99
Mg^{2+}	12-6 CM	TIP4P-FB	-76.54	1.91
Mg^{2+}	12-6-4	TIP4P-FB	-77.05	1.99
Mg^{2+}	Drude oscillator model[a]	SWM4-NDP[a]	-89.4	1.86
Mg^{2+}	AMOEBA[b]	AMOEBA[b]	-79.56	1.88
Mg^{2+}	ωB97X-V/def2-QZVPPD[b]	N/A	-83.12	1.91
Ca^{2+}-H_2O dimer				
Ca^{2+}	12-6 HFE	OPC	-67.03	2.17
Ca^{2+}	12-6 IOD	OPC	-59.09	2.32
Ca^{2+}	12-6 CM	OPC	-57.82	2.34
Ca^{2+}	12-6-4	OPC	-61.29	2.31
Ca^{2+}	12-6 HFE	TIP3P-FB	-58.13	2.21
Ca^{2+}	12-6 IOD	TIP3P-FB	-51.97	2.34
Ca^{2+}	12-6 CM	TIP3P-FB	-50.93	2.37
Ca^{2+}	12-6-4	TIP3P-FB	-53.89	2.35
Ca^{2+}	12-6 HFE	TIP4P-FB	-61.30	2.16
Ca^{2+}	12-6 IOD	TIP4P-FB	-53.24	2.33
Ca^{2+}	12-6 CM	TIP4P-FB	-51.61	2.37
Ca^{2+}	12-6-4	TIP4P-FB	-55.37	2.34
Ca^{2+}	Drude oscillator model[a]	SWM4-NDP[a]	-55.6	2.18
Ca^{2+}	AMOEBA[b]	AMOEBA[b]	-54.65	2.22
Ca^{2+}	ωB97X-V/def2-QZVPPD[b]	N/A	-57.97	2.22

[a]From Ref.[2]; [b]From Ref.[3].

Table S11. Reaction Energies for the $[Zn(H_2O)_n]^{2+} + H_2O \rightarrow [Zn(H_2O)_{n+1}]^{2+}$ Reaction[a]

Set	Water Model	$n = 0$	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	AUE
12-6 HFE	OPC3	-104.04	-98.08	-82.95	-64.69	-29.28	-14.90	12.63
12-6 IOD	OPC3	-71.80	-68.53	-62.07	-55.25	-40.14	-37.12	11.00
12-6 CM	OPC3	-88.42	-83.88	-74.05	-62.73	-32.21	-33.36	6.97
12-6-4	OPC3	-79.12	-75.92	-69.59	-62.90	-47.90	-44.45	13.59
12-6 HFE	OPC	-124.70	-115.03	-88.21	-59.66	-31.88	-31.39	16.79
12-6 IOD	OPC	-80.43	-75.82	-66.84	-57.58	-37.30	-34.67	8.65
12-6 CM	OPC	-107.27	-99.91	-82.90	-63.74	-31.03	-10.95	13.68
12-6-4	OPC	-88.14	-83.74	-75.15	-66.27	-46.66	-43.17	11.86
12-6 HFE	TIP3P-FB	-104.93	-98.98	-82.76	-63.08	-29.06	-9.74	13.53
12-6 IOD	TIP3P-FB	-69.44	-66.42	-60.43	-54.05	-39.83	-36.91	11.20
12-6 CM	TIP3P-FB	-85.97	-81.73	-72.48	-61.68	-31.98	-33.27	7.25
12-6-4	TIP3P-FB	-77.29	-74.34	-68.50	-62.27	-48.21	-44.88	14.00
12-6 HFE	TIP4P-FB	-113.99	-106.50	-83.89	-58.64	-29.94	-28.25	12.51
12-6 IOD	TIP4P-FB	-71.55	-68.17	-61.48	-54.40	-38.42	-35.77	10.35
12-6 CM	TIP4P-FB	-93.44	-88.23	-76.19	-61.97	-24.15	-28.76	6.74
12-6-4	TIP4P-FB	-80.08	-76.80	-70.37	-63.54	-47.97	-44.70	13.58
QM[b]	N/A	-95.10	-85.86	-60.48	-48.53	-31.18	-29.01	0.00

[a]Unit is kcal/mol. Depending on the parameters and water model, the optimized structure may not have all the water molecules in the first coordination shell.

[b]The QM calculations were performed at the MP4SDQ(FC)/HUZSP*//RHF/HUZSP* level of theory[4].

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