Supporting Information for

Impacts of targeting different hydration free energy references on the development of ion potentials

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Table S1. System Size and Composition for All of the Simulations in This Work

system	box size (Å³)	composition	note
ion solution	26.4 x 26.4 x 26.4	1 ion + 600 water	HFE, IOD, and ion diffusion
	31.5 x 31.4 x 31.5	1 ion + 1024 water	water exchange rate
	40 x 40 x 40	8 K^+ + 8 Cl^- + 2149 water	0.2 mol/L KCl
	40 x 40 x 40	58 K^+ + 58 Cl^- + 2049 water	1.5 mol/L KCl
	40 x 40 x 40	116 K^+ + 116 Cl^- + 1933 water	3.0 mol/L KCl
	40 x 40 x 40	8 Mg^{2+} + 16 Cl^- + 2141 water	0.2 mol/L $MgCl_2$
	40 x 40 x 40	58 Mg^{2+} + 116 Cl^- + 1991 water	1.5 mol/L $MgCl_2$
	40 x 40 x 40	116 Mg^{2+} + 232 Cl^- + 1817 water	3.0 mol/L $MgCl_2$
	40 x 40 x 40	8 Al^{3+} + 24 Cl^- + 2133 water	0.2 mol/L $AlCl_3$
	40 x 40 x 40	58 Al^{3+} + 174 Cl^- + 1933 water	1.5 mol/L $AlCl_3$
	40 x 40 x 40	116 Al^{3+} + 348 Cl^- + 1701 water	3.0 mol/L $AlCl_3$
	40 x 40 x 80	8 K^+ + 8 Cl^- + 4314 water	0.2 mol/L KCl (osmotic pressure)
	40 x 40 x 80	19 K^+ + 19 Cl^- + 4292 water	0.5 mol/L KCl (osmotic pressure)
	40 x 40 x 80	39 K^+ + 39 Cl^- + 4252 water	1.0 mol/L KCl (osmotic pressure)
	40 x 40 x 80	58 K^+ + 58 Cl^- + 4214 water	1.5 mol/L KCl (osmotic pressure)
	40 x 40 x 80	77 K^+ + 77 Cl^- + 4176 water	2.0 mol/L KCl (osmotic pressure)
	40 x 40 x 80	96 K^+ + 96 Cl^- + 4318 water	2.5 mol/L KCl (osmotic pressure)
	40 x 40 x 80	116 K^+ + 116 Cl^- + 4098 water	3.0 mol/L KCl (osmotic pressure)
	40 x 40 x 80	135 K^+ + 135 Cl^- + 4060 water	3.5 mol/L KCl (osmotic pressure)
	40 x 40 x 80	8 Mg^{2+} + 16 Cl^- + 4306 water	0.2 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	19 Mg^{2+} + 39 Cl^- + 4273 water	0.5 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	39 Mg^{2+} + 78 Cl^- + 4213 water	1.0 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	58 Mg^{2+} + 116 Cl^- + 4156 water	1.5 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	77 Mg^{2+} + 154 Cl^- + 4111 water	2.0 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	96 Mg^{2+} + 192 Cl^- + 4066 water	2.5 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	116 Mg^{2+} + 232 Cl^- + 4018 water	3.0 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	135 Mg^{2+} + 279 Cl^- + 3978 water	3.5 mol/L $MgCl_2$ (osmotic pressure)
	40 x 40 x 80	8 Al^{3+} + 24 Cl^- + 4298 water	0.2 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	19 Al^{3+} + 57 Cl^- + 4254 water	0.5 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	39 Al^{3+} + 117 Cl^- + 4199 water	1.0 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	58 Al^{3+} + 174 Cl^- + 4159 water	1.5 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	77 Al^{3+} + 231 Cl^- + 4121 water	2.0 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	96 Al^{3+} + 288 Cl^- + 4067 water	2.5 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	116 Al^{3+} + 348 Cl^- + 4010 water	3.0 mol/L $AlCl_3$ (osmotic pressure)
	40 x 40 x 80	135 Al^{3+} + 405 Cl^- + 3963 water	3.5 mol/L $AlCl_3$ (osmotic pressure)
ion pair	vacuum	1 K^+ + 1 Cl^-	
salt crystal	31.5 x 31.5 x 31.5	500 K^+ + 500 Cl^-	
salt melting	31.5 x 31.5 x 70.5	1000 K^+ + 1000 Cl^-	
metalloprotein	74.1 x 68.4 x 77.7	1 protein + 1 Mg^{2+} + 4 Na^+ + 9345 water	

Table S2. Comparison of Calculated Water Exchange Rates (k_1, s^{-1}) in the First Hydration Shell of Mg^{2+} Ion from MD Simulations in TIP3P Water Using the Methods of Exchange Number Count and Transition State Theory

model	exchange number count	transition state theory
*micro*Mg[a]	$(8.04 \pm 1.20) \times 10^{5a}$	7.2×10^6 (this work)
*nano*Mg[a]	$(1.11 \pm 0.003) \times 10^{8a}$	2.9×10^8 (this work)
Mamatkulov−Schwierz[b]	24.0 ± 8.8^{b}	4.3×10^3 (this work)
Allnér et al.[c]	NA	6.8×10^{5c}, 2.4×10^{5a}, 6.1×10^{5d}
Li−Merz (12−6 HFE)[e]	NA	3.5×10^{4a}, 5.4×10^{3f}
Li−Merz (12−6-4)[e]	$(1.44 \pm 0.03) \times 10^{7a}$	1.19×10^{8g}
exp	$(6.7 \pm 0.2) \times 10^{5h}$	$(6.7 \pm 0.2) \times 10^{5h}$

[a]Taken from Grotz et al.[1] [b]From Ref.[2] [c]From Ref.[3] [d]From Ref.[4] [e]From Ref.[5, 6] [f]From Ref.[7] [g]From Ref.[8] [h]From Ref.[9] NA means that the number of transitions is insufficient to calculate the rate.[1]

Table S3. Calculated Osmotic Pressure (Π, bar) and Osmotic Coefficient (φ) of KCl Solutions Using Different Ion Models[a]

molarity	KCl(-5)			KCl(0)			KCl(+5)		
	Π	φ	exp	Π	φ	exp	Π	φ	exp
0.2	11.60 ± 0.80	1.16 ± 0.08	0.91	9.60 ± 0.80	0.96 ± 0.08	0.91	9.80 ± 0.70	0.98 ± 0.07	0.91
0.5	22.40 ± 0.80	0.89 ± 0.03	0.90	23.30 ± 1.00	0.93 ± 0.04	0.90	20.70 ± 0.90	0.82 ± 0.04	0.90
1.0	51.00 ± 2.10	1.00 ± 0.04	0.90	45.10 ± 1.10	0.89 ± 0.02	0.90	46.10 ± 1.20	0.91 ± 0.02	0.90
1.5	84.30 ± 2.00	1.09 ± 0.03	0.90	66.90 ± 1.40	0.86 ± 0.02	0.90	65.30 ± 2.00	0.84 ± 0.03	0.90
2.0	114.40 ± 3.20	1.09 ± 0.03	0.91	88.30 ± 2.10	0.84 ± 0.02	0.91	83.90 ± 3.00	0.80 ± 0.03	0.91
2.5	150.00 ± 2.30	1.13 ± 0.02	0.92	111.30 ± 2.50	0.84 ± 0.02	0.92	102.40 ± 2.00	0.77 ± 0.01	0.92
3.0	192.80 ± 4.50	1.19 ± 0.03	0.93	137.30 ± 2.50	0.85 ± 0.01	0.93	117.30 ± 3.00	0.73 ± 0.02	0.93
3.5	242.60 ± 4.00	1.27 ± 0.02	0.94	150.20 ± 2.30	0.79 ± 0.01	0.94	136.70 ± 4.10	0.71 ± 0.01	0.94
RMSE		0.21			0.07			0.13	
MAE		0.19			0.06			0.11	
MSE		0.19			-0.04			-0.09	

molarity	KCl(JC)			KCl(Roux)			KCl(Zhang)		
	Π	Φ	exp	Π	Φ	exp	Π	φ	exp
0.2	10.10 ± 0.60	1.01 ± 0.06	0.91	9.30 ± 0.70	0.93 ± 0.07	0.91	7.50 ± 0.50	0.75 ± 0.05	0.91
0.5	21.20 ± 0.90	0.84 ± 0.04	0.90	22.50 ± 1.20	0.90 ± 0.05	0.90	13.30 ± 1.10	0.53 ± 0.04	0.90
1.0	44.70 ± 1.10	0.88 ± 0.02	0.90	47.70 ± 1.20	0.94 ± 0.02	0.90	19.30 ± 1.60	0.38 ± 0.03	0.90
1.5	73.70 ± 1.70	0.95 ± 0.02	0.90	73.30 ± 1.70	0.95 ± 0.02	0.90	14.80 ± 1.10	0.19 ± 0.01	0.90
2.0	94.50 ± 2.20	0.90 ± 0.02	0.91	90.10 ± 1.70	0.86 ± 0.02	0.91	17.30 ± 1.20	0.17 ± 0.01	0.91
2.5	120.30 ± 2.30	0.91 ± 0.02	0.92	117.90 ± 2.10	0.89 ± 0.02	0.92	14.70 ± 1.90	0.11 ± 0.01	0.92
3.0	137.60 ± 2.10	0.85 ± 0.01	0.93	151.20 ± 3.10	0.94 ± 0.02	0.93	11.00 ± 1.20	0.07 ± 0.01	0.93
3.5	165.70 ± 3.30	0.87 ± 0.02	0.94	168.90 ± 2.80	0.88 ± 0.01	0.94	14.30 ± 1.10	0.07 ± 0.01	0.94
RMSE		0.06			0.04			0.67	
MAE		0.05			0.03			0.63	
MSE		-0.01			0.00			-0.63	

[a]Experimental osmotic coefficients were taken from polynomial fits of the reported data as a function of molality.[10] Density of salt solutions[11, 12] was used to convert the concentration between molarity and molality.

Table S4. Calculated Osmotic Pressure (Π, bar) and Osmotic Coefficient (φ) of MgCl$_2$ Solutions Using Different Ion Models[a]

molarity	MgCl$_2$(-5)			MgCl$_2$(0)			MgCl$_2$(+5)		
	Π	φ	exp	Π	φ	exp	Π	φ	exp
0.2	13.30 ± 1.00	0.89 ± 0.07	0.88	11.50 ± 0.90	0.77 ± 0.06	0.88	13.10 ± 0.80	0.87 ± 0.05	0.88
0.5	31.30 ± 1.50	0.83 ± 0.04	0.94	24.80 ± 1.30	0.66 ± 0.04	0.94	23.90 ± 1.50	0.64 ± 0.04	0.94
1.0	72.00 ± 2.50	0.95 ± 0.03	1.09	54.90 ± 2.30	0.73 ± 0.03	1.09	31.00 ± 1.80	0.41 ± 0.02	1.09
1.5	108.50 ± 2.40	0.95 ± 0.02	1.25	76.90 ± 2.10	0.67 ± 0.02	1.25	34.80 ± 1.60	0.30 ± 0.01	1.25
2.0	165.10 ± 4.20	1.07 ± 0.03	1.42	93.80 ± 3.50	0.61 ± 0.02	1.42	36.90 ± 5.10	0.24 ± 0.03	1.42
2.5	204.90 ± 5.90	1.06 ± 0.03	1.59	105.80 ± 3.30	0.55 ± 0.02	1.59	41.70 ± 3.50	0.22 ± 0.02	1.59
3.0	276.50 ± 3.90	1.18 ± 0.02	1.76	137.30 ± 5.00	0.59 ± 0.02	1.76	38.40 ± 2.30	0.16 ± 0.01	1.76
3.5	329.40 ± 5.00	1.20 ± 0.02	1.93	136.80 ± 4.10	0.50 ± 0.01	1.93	43.50 ± 3.80	0.16 ± 0.01	1.93
RMSE		0.42			0.84			1.14	
MAE		0.34			0.72			0.98	
MSE		-0.34			-0.72			-0.98	

molarity	MgCl$_2$(+10)			MgCl$_2$(+15)		
	Π	φ	exp	Π	φ	exp
0.2	10.30 ± 0.80	0.69 ± 0.05	0.88	4.50 ± 0.70	0.30 ± 0.05	0.88
0.5	11.50 ± 1.30	0.31 ± 0.04	0.94	1.80 ± 0.40	0.05 ± 0.01	0.94
1.0	7.40 ± 0.80	0.10 ± 0.01	1.09	0.90 ± 0.20	0.01 ± 0.00	1.09
1.5	4.90 ± 0.70	0.04 ± 0.01	1.25	0.90 ± 0.20	0.01 ± 0.00	1.25
2.0	5.80 ± 1.20	0.04 ± 0.01	1.42	0.90 ± 0.50	0.01 ± 0.00	1.42
2.5	4.90 ± 0.90	0.03 ± 0.01	1.59	1.40 ± 0.40	0.01 ± 0.00	1.59
3.0	2.80 ± 0.40	0.01 ± 0.00	1.76	0.20 ± 0.10	0.00 ± 0.00	1.76
3.5	2.50 ± 0.40	0.01 ± 0.00	1.93	0.40 ± 0.20	0.00 ± 0.00	1.93
RMSE		1.32			1.37	
MAE		1.20			1.31	
MSE		-1.20			-1.31	

[a]Experimental osmotic coefficients were taken from polynomial fits of the reported data as a function of molarity.[13] Density of salt solutions[13] was used to convert the concentration between molarity and molality.

Table S5. Calculated Osmotic Pressure (Π, bar) and Osmotic Coefficient (φ) of AlCl$_3$ Solutions Using Different Ion Models[a]

molarity	AlCl$_3$(-5)			AlCl$_3$(0)			AlCl$_3$(+5)		
	Π	φ	exp	Π	φ	exp	Π	φ	exp
0.2	16.10 ± 0.90	0.81 ± 0.04	0.85	9.60 ± 1.00	0.48 ± 0.05	0.85	2.40 ± 0.60	0.12 ± 0.03	0.85
0.5	37.50 ± 1.20	0.75 ± 0.02	0.98	12.20 ± 1.00	0.24 ± 0.02	0.98	4.80 ± 0.80	0.10 ± 0.02	0.98
1.0	65.30 ± 2.70	0.65 ± 0.03	1.30	8.70 ± 1.20	0.09 ± 0.01	1.30	1.30 ± 0.40	0.01 ± 0.00	1.30
1.5	100.00 ± 3.00	0.66 ± 0.02	1.67	11.10 ± 1.60	0.07 ± 0.01	1.67	1.20 ± 0.90	0.01 ± 0.01	1.67
2.0	103.70 ± 5.80	0.51 ± 0.03	2.08	10.10 ± 0.80	0.05 ± 0.00	2.08	0.90 ± 0.40	0.01 ± 0.00	2.08
2.5	140.70 ± 4.20	0.56 ± 0.02	2.55	13.60 ± 1.00	0.05 ± 0.00	2.55	0.50 ± 0.20	0.00 ± 0.00	2.55
3.0	140.00 ± 9.10	0.46 ± 0.03	3.02	18.90 ± 2.50	0.06 ± 0.01	3.02	0.20 ± 0.10	0.00 ± 0.00	3.02
3.5	172.00 ± 9.00	0.48 ± 0.03	3.38	19.40 ± 2.60	0.05 ± 0.01	3.38	0.60 ± 0.10	0.00 ± 0.00	3.38
RMSE	1.69			2.09			2.15		
MAE	1.37			1.84			1.95		
MSE	-1.37			-1.84			-1.95		

molarity	AlCl$_3$(+10)			AlCl$_3$(+15)		
	Π	φ	exp	Π	φ	exp
0.2	0.40 ± 0.20	0.02 ± 0.01	0.85	2.70 ± 0.90	0.14 ± 0.04	0.85
0.5	0.50 ± 0.20	0.01 ± 0.00	0.98	0.40 ± 0.30	0.01 ± 0.01	0.98
1.0	0.10 ± 0.10	0.00 ± 0.00	1.30	0.00 ± 0.00	0.00 ± 0.00	1.30
1.5	0.00 ± 0.00	0.00 ± 0.00	1.67	0.00 ± 0.00	0.00 ± 0.00	1.67
2.0	0.00 ± 0.00	0.00 ± 0.00	2.08	0.00 ± 0.00	0.00 ± 0.00	2.08
2.5	0.00 ± 0.00	0.00 ± 0.00	2.55	0.00 ± 0.00	0.00 ± 0.00	2.55
3.0	0.00 ± 0.00	0.00 ± 0.00	3.02	0.00 ± 0.00	0.00 ± 0.00	3.02
3.5	0.00 ± 0.00	0.00 ± 0.00	3.38	0.00 ± 0.00	0.00 ± 0.00	3.38
RMSE	2.17			2.16		
MAE	1.98			1.96		
MSE	-1.98			-1.96		

[a]Experimental osmotic coefficients were taken from polynomial fits of the reported data as a function of molarity.[14, 15] Density of salt solutions[15] was used to convert the concentration between molarity and molality.

Table S6. Simulated Mg─N and Mg─O Distances (Å) for the Different Mg²⁺ Models Calculated from Protein 5TKA Simulations Using the Amber ff14SB Force Field with Original and Modified Atomic Charges of Asp67 and Asp132[a]

model	H31_NE2	H66_NE2	D67_OD1	D67_OD2	D132_OD1	D132_OD2	W1	W2[b]
				original Asp (identical charges for OD1/OD2)				
Mg(-5)	2.33 ± 0.08	2.22 ± 0.06	2.07 ± 0.05	2.04 ± 0.05	2.04 ± 0.05	2.08 ± 0.06	2.12 ± 0.05	30.06 ± 9.45
Mg(0)	2.36 ± 0.09	2.22 ± 0.06	2.08 ± 0.06	2.03 ± 0.05	2.04 ± 0.05	2.08 ± 0.07	2.12 ± 0.05	34.02 ± 9.33
Mg(+5)	2.36 ± 0.10	2.25 ± 0.07	2.08 ± 0.06	2.04 ± 0.05	2.10 ± 0.07	2.05 ± 0.06	2.13 ± 0.05	34.28 ± 9.04
Mg(+10)	2.37 ± 0.13	2.26 ± 0.08	2.09 ± 0.07	2.04 ± 0.06	2.29 ± 0.55	2.06 ± 0.19	2.11 ± 0.05	31.16 ± 8.90
Mg(+15)	2.40 ± 0.24	2.25 ± 0.07	2.69 ± 0.64	2.19 ± 0.42	2.00 ± 0.04	3.85 ± 0.15	2.13 ± 0.06	33.69 ± 10.97
				modified Asp (different charges for OD1/OD2)				
Mg(-5)	2.33 ± 0.08	2.24 ± 0.06	2.11 ± 0.06	2.00 ± 0.04	2.03 ± 0.05	2.07 ± 0.08	2.13 ± 0.05	4.15 ± 0.30
Mg(0)	2.30 ± 0.11	2.23 ± 0.06	2.46 ± 0.56	1.98 ± 0.04	1.99 ± 0.06	2.61 ± 0.77	2.13 ± 0.05	33.30 ± 8.39
Mg(+5)	2.23 ± 0.09	2.23 ± 0.06	2.78 ± 0.65	1.98 ± 0.05	1.96 ± 0.04	3.72 ± 0.44	2.12 ± 0.05	2.12 ± 0.05
Mg(+10)	2.23 ± 0.07	2.26 ± 0.07	3.42 ± 0.18	1.96 ± 0.04	1.94 ± 0.04	3.73 ± 0.16	2.13 ± 0.06	2.13 ± 0.06
Mg(+15)	2.25 ± 0.07	2.27 ± 0.08	3.70 ± 0.21	1.96 ± 0.04	1.96 ± 0.04	3.85 ± 0.13	2.14 ± 0.06	2.15 ± 0.06
crystal	2.24	2.21	3.30	2.09	2.12	3.93	1.94	1.92

[a]The atoms with a Mg─O distances of > 2.5 Å are not considered in the calculation of the coordination number of Mg²⁺ and are marked in red.

[b]A larger distance of > 2.5 Å indicates than the crystal binding water moves away from the metal binding center, and due to the bidentate poses of Asp residues, no additional water molecules enter into the metal binding sphere in most cases.
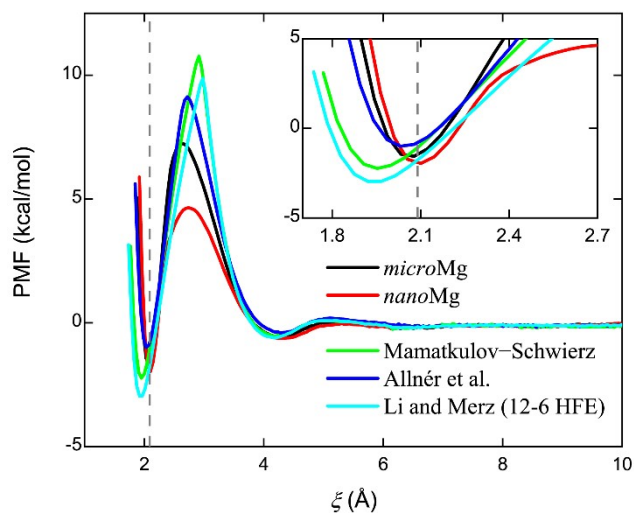
Figure S1. Potential of mean force (PMF) profiles of Mg^{2+} binding to one water molecule in TIP3P aqueous solution as a function of the distance (ξ) between the ion and water oxygen atom (i.e., IOD). The dashed line represents the experimental IOD of 2.09 Å. Refer to Table S1 for different Mg^{2+} models.
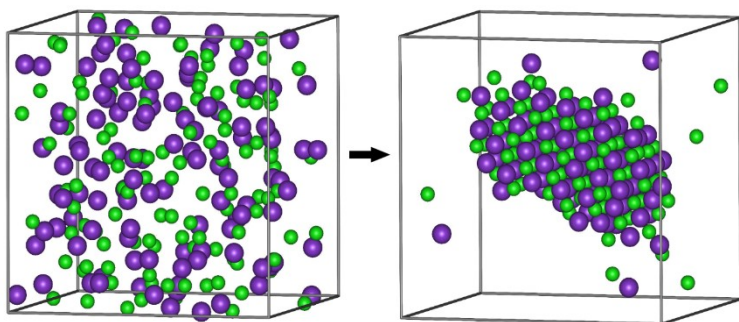

Figure S2. KCl crystallization at 3.0 mol/L salt solution during MD simulations using the ion models by Roux et al.[16] Water molecules are not shown here for clarity. Purple balls represent K^+ ions and green ones are for Cl^- ions.
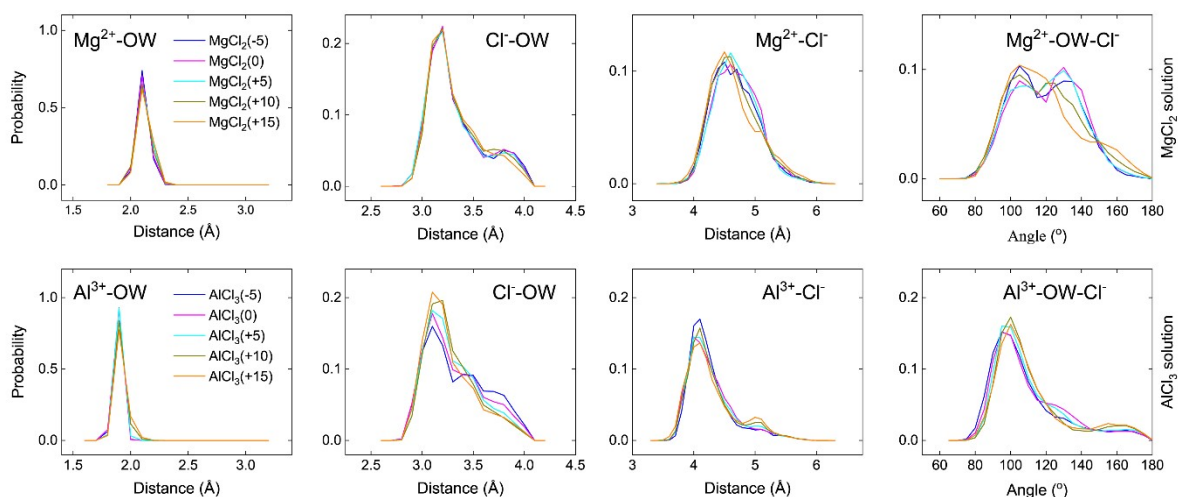
Figure S3. Distribution for the ion–water and ion–ion distances and the cation–water–anion angles for the structures with one bridging water existing between the cation and the anion for MgCl₂ (*top)* and AlCl₃ (*bottom*) solutions. Ten frames with an interval of 2 ns from the last 20 ns trajectories were used for the calculation, excluding the conformations in which the cation binds to the anion within its first solvation shell.
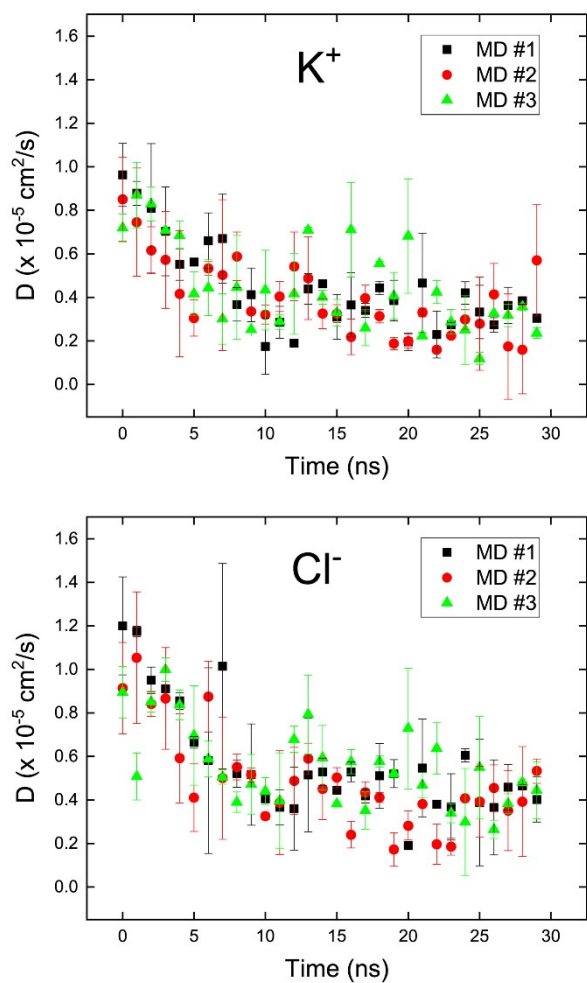
Figure S4. Diffusion constants of K$^+$ and Cl$^-$ ions in the simulation of aqueous salt solutions with a concentration of 3.0 mol/L using the ion models by Roux et al.[16] Three independent MD simulations were performed with different initial velocities.
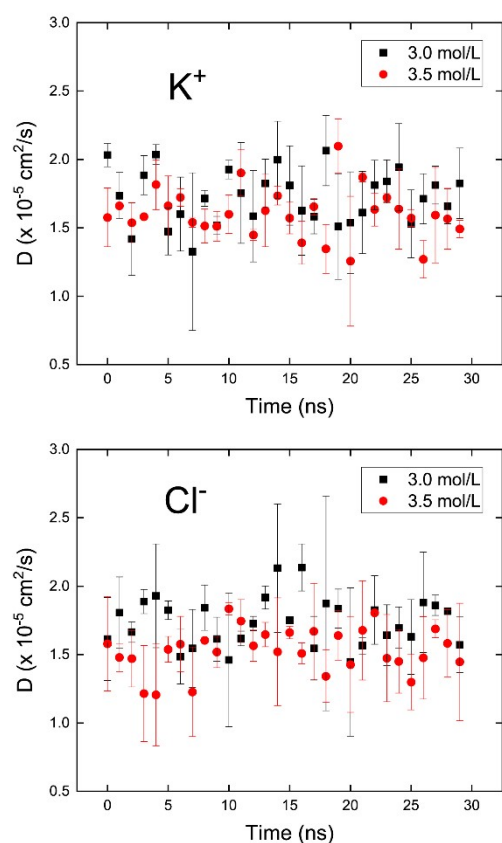
Figure S5. Diffusion constants of K^+ and Cl^- ions in the simulation of osmotic pressure for KCl salt solutions at concentrations of 3.0 and 3.5 mol/L using the ion models by Roux et al.[16]
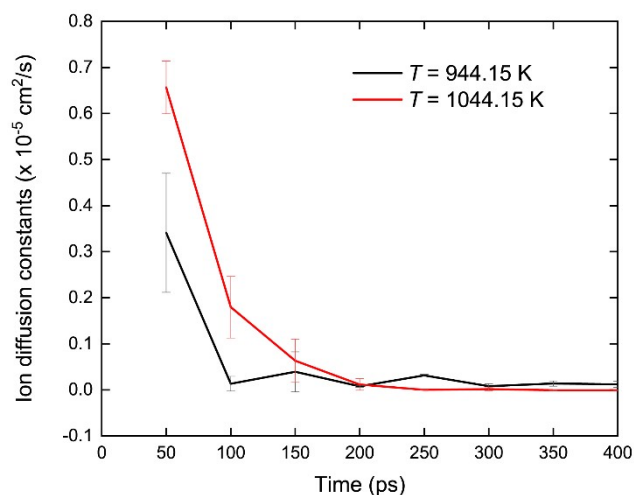

Figure S6. Jump in the ion diffusion constants of KCl salts for the transition a liquid-solid direct coexistence state to a solid crystal in the 400-ps NPT simulations at 944.15 and 1044.15 K using the ion models by Joung–Cheatham et al.[17]
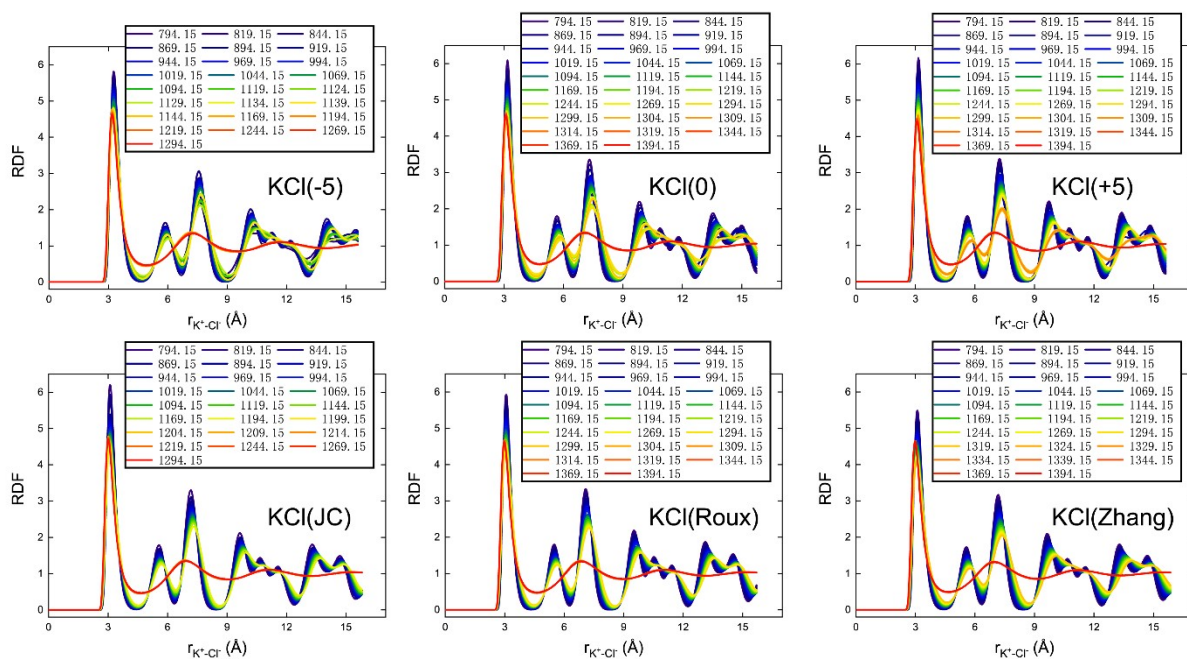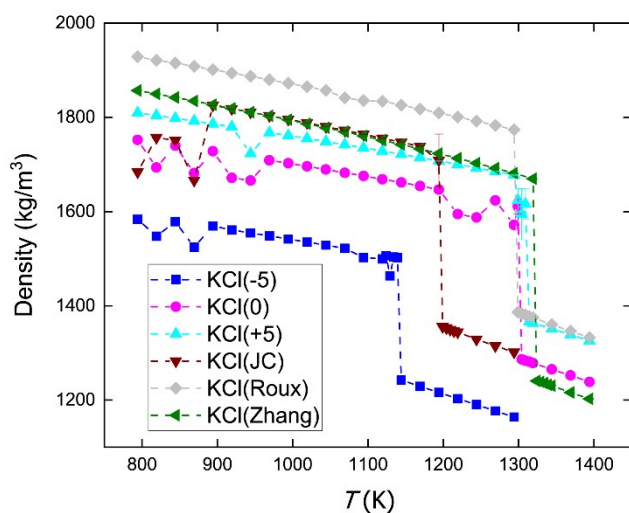
Figure S7. Cation–anion RDFs for the simulated KCl salts at different temperatures using a liquid-solid direct coexistence state as an initial configuration.
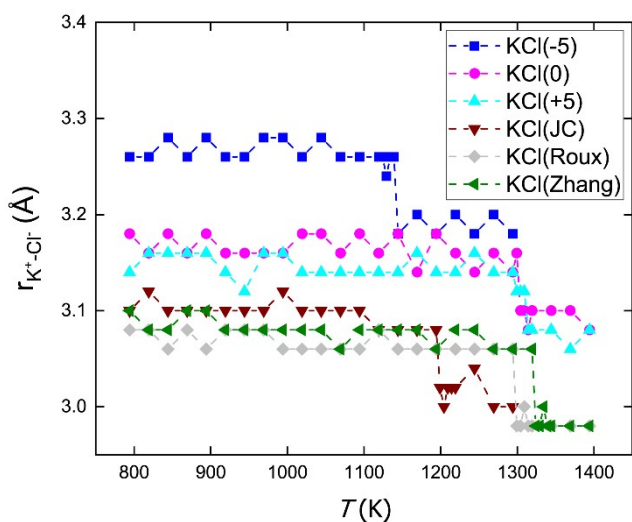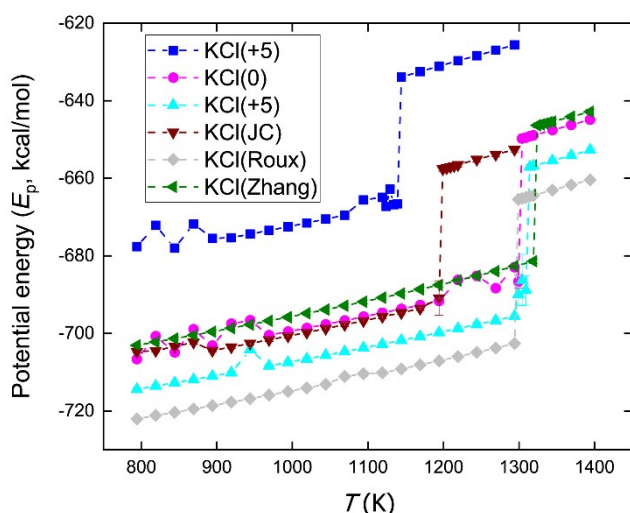

Figure S8. Changes in the cation–anion distances for the first peaks of the cation–anion RDFs for the simulated KCl salts at different temperatures using a liquid-solid direct coexistence state as an initial configuration.
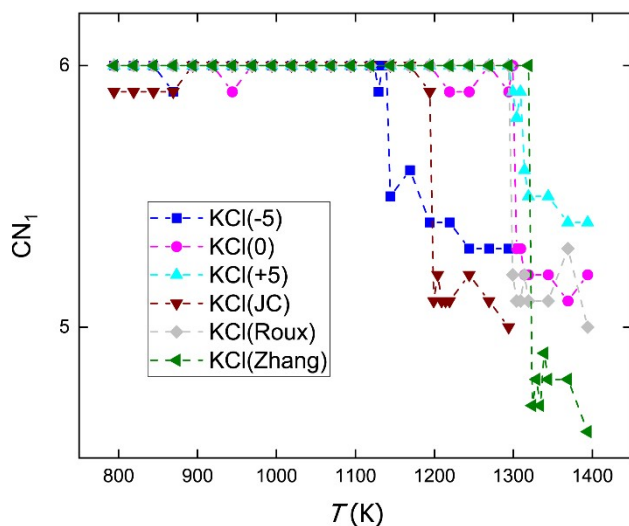
Figure S9. Changes in the coordination number for the first peaks of the cation–anion RDFs for the simulated KCl salts at different temperatures using a liquid-solid direct coexistence state as an initial configuration

Figure S10. Changes in the density of the simulated KCl salts at different temperatures using a liquid-solid direct coexistence state as an initial configuration

Figure S11. Changes in the potential energy per ion pair (E_p) of the simulated KCl salts at different temperatures using a liquid-solid direct coexistence state as an initial configuration

References

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