SUPPORTING INFORMATION

Creating water-in-salt-like environment using strongly coordinating anions in non-concentrated aqueous electrolytes for efficient Zn batteries

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1. SUPPLEMENTARY TABLES 1-4

Table S1. Measured and molecular dynamics (MD) predicted physicochemical properties of the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes

Electrolyte	Viscosity (experimental) mPa s	Density (experimental) g cm^{-3}	Density (MD) g cm^{-3}	Conductivity (experimental) mS cm^{-1}	Conductivity (MD) mS cm^{-1}	Conductivity (Molar, exp.) S cm^2 mol^{-1}
$Zn_{0.2}K_{0.8}Oac_{1.2}$ $50H_2O$	1.3	1.06	1.07	59.3	64.4	63.24
$Zn_{0.2}K_{0.8}OAc_{1.2}$ $20H_2O$	1.7	1.13	1.13	89.2	91.6	47.86
$Zn_{0.2}K_{0.8}OAc_{1.2}$ $10H_2O$	2.9	1.22	1.22	90.0	86.6	32.13
$Zn_{0.2}K_{0.8}OAc_{1.2}$ $5H_2O$	9	1.33	1.31	60.2	61.6	16.41
$Zn_{0.2}K_{0.8}OAc_{1.2}$ $2H_2O$	81.2	1.47	1.41	14.2	11.7	3.14
$Zn_{0.2}K_{0.8}OAc_{1.2}$ $1.5H_2O$	268.9	1.50	1.43	5.4	4.7	1.15
$ZnOAc_2$ $42H_2O$	-	-	-	17.8	-	-

Table S2. EXAFS fitting parameters and results for the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O with n= 50 and 2 to different DFT models. The parameters in the table are the water content *n*, the DFT model fraction *x*, coordination number (CN), the radial distance *R*, the Debye-Waller factor σ^2, and the edge energy uncertainty ΔE. The amplitude reduction factor S_0^2, is consider constant with a value of 1 based in previously reported literature.[1]

Water content "n"	DFT Model	Scattering path	Fraction "x"	error on x	CN	R (Å) Abs	error on R	σ^2 (Å^2)	error on σ^2	ΔE	error on ΔE	R-value	R range	k range
50	$Zn(H_2O)_6$	Zn-Ow			6	2.0804		0.0147	0.0015	9.11	1.10	0.08	1.2-3	3 to 12
50	$Zn(OAc)_4$ - mono	Zn-OAc			4	1.9785		0.0081	0.0013	-4.16	1.95	0.12	1.2-3	3 to 12
50	$Zn(OAc)_2$-$(H_2O)_4$ - mono	Zn-OAc Zn-Ow			2 4	2.0273 2.1535		0.0049 0.0175	0.0009 0.0024	10.08	0.91	0.03	1.2-3	3 to 12
50	**$Zn(H_2O)_6$** **$Zn(OAc)_4$ - mono**	**Zn-Ow** **Zn-OAc**	**0.658** **0.342**	**0.173** **0.173**	**6** **4**	**2.0804** **1.9785**		**0.0118** **0.0053**	**0.0022** **0.0005**	**5.36**	**0.80**	**0.02**	**1.2-3**	**3 to 12**
2	$Zn(H_2O)_6$	Zn-Ow			6	2.0804		0.0170	0.0049	16.14	2.75	0.40	1.2-3	3 to 12
2	**$Zn(OAc)_4$ - mono**	**Zn-OAc**			**4**	**1.9785**		**0.0058**	**0.0005**	**5.67**	**0.74**	**0.02**	**1.2-3**	**3 to 12**
2	$Zn(OAc)_2$-$(H_2O)_4$ - mono	Zn-OAc Zn-Ow			2 4	2.0273 2.1535		0.0031 0.0305	0.0020 0.0167	16.46	2.58	0.18	1.2-3	3 to 12
2	$Zn(H_2O)_6$ $Zn(OAc)_4$ - mono	Zn-Ow Zn-OAc	-0.002 1.002	0.006 0.006	6 4	2.0804 1.9785		-0.0121 0.0061	0.0127 0.0007	5.49	0.90	0.02	1.2-3	3 to 12
2	$Zn(OAc)_4$ - mono	Zn-O Zn-C-O Zn-O			4 4 4	1.9639 3.1132 4.1403	0.0053 0.0321 0.0385	0.0056 0.0018 0.0100	0.0003 0.0043 0.0051	2.90	1.06	0.0143	1.2 to 4.5	3 to 12

Table S3. EXAFS fitting parameters and results of the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes to the combination of x_n $Zn(H_2O)_6^{2+}$ octahedral and $(1-x_n)$ $Zn(OAc)_4^{2-}$ tetrahedral DFT generated models. The DFT model fractions (x_n) were generated from the best fits to the electrolytes n=50 and n=2 (input rows from Table 2) and the linear combination fitting results from Figure S9 b. The parameters in the table are the water content *n*, the linear combination fitting (LCF) results *y*, coordination number (CN), the radial distance *R*, the Debye-Waller factor σ^2, and the edge energy uncertainty ΔE. The Amplitude reduction factor S_0^2 is considered constant with a value of 1 based on previously reported literature.[1]

	Water content "n"	LCF "y"	DFT Model	Fraction "x_n $(1-x_n)$"	Scattering path	CN	R (Å) Abs	σ^2 (Å^2)	error on σ^2	ΔE	error on ΔE	R-value	R range	k range
Input	**50**	**0**	**Zn(H2O)6** **Zn(OAc)4 - mono**	**0.657** **0.342**	**Zn-Ow** **Zn-OAc**	**6** **4**	**2.0804** **1.9785**	**0.0112** **0.0049**	**0.0024** **0.0024**	**5.48**	**1.45**	**0.02**	**1.2-3**	**3 to 12**
	30	0.292	Zn(H2O)6 Zn(OAc)4 - mono	0.455 0.545	Zn-Ow Zn-OAc	6 4	2.0804 1.9785	0.0106 0.0053	0.0012 0.0006	5.24	0.69	0.01	1.2-3	3 to 12
	20	0.487	Zn(H2O)6 Zn(OAc)4 - mono	0.332 0.668	Zn-Ow Zn-OAc	6 4	2.0804 1.9785	0.0118 0.0053	0.0022 0.0005	5.36	0.80	0.02	1.2-3	3 to 12
	10	0.731	Zn(H2O)6 Zn(OAc)4 - mono	0.174 0.826	Zn-Ow Zn-OAc	6 4	2.0804 1.9785	0.0131 0.0056	0.0063 0.0005	5.77	0.94	0.02	1.2-3	3 to 12
	5	0.909	Zn(H2O)6 Zn(OAc)4 - mono	0.065 0.935	Zn-Ow Zn-OAc	6 4	2.0804 1.9785	0.0056 0.0176	0.0303 0.0004	5.88	1.00	0.01	1.2-3	3 to 12
Input	**2**	**1**	**Zn(OAc)4 - mono**	**1**	**Zn-OAc**	**4**	**1.9785**	**0.0058**	**0.0005**	**5.67**	**0.74**	**0.02**	**1.2-3**	**3 to 12**

Table S4. Binding energies for 16 species from density functional theory (E^{QM}) computed at the counterpoise-corrected ωB97X-D/6-311++G(3df,3pd) level of theory in the gas phase compared against binding energies from force field iteration 1 (E^{FF1}) and iteration 2 (E^{FF2}). For clarity the negative of the binding energies is used ($-E^{QM}$, for example). The unsigned errors ($|\Delta|$) between the density functional and force field result are reported and the mean unsigned error is listed at the bottom of the relevant column. All energies in kcal/mol which is the native energy unit in Tinker. Ignoring the highest error species 9-11, the mean unsigned error in FF1 is 3.44 kcal/mol. The main effect of the refitting is to lessen Zn-OAc aggregation, resulting in inflated conductivities versus experiment. Thus, all results unless otherwise noted reflect FF1 only.

No.	**Species**	$-E^{QM}$	$-E^{FF1}$	$\|\Delta\|_{FF1}$	$-E^{FF2}$	$\|\Delta\|_{FF2}$
1	$[OAc(H_2O)]^-$	20.82	18.82	2.00	19.59	1.23
2	$[OAc(H_2O)_2]^-$	34.78	31.91	2.87	33.85	0.93
3	$[OAc(H_2O)_3]^-$	46.18	42.23	3.95	45.12	1.06
4	$[OAc(H_2O)_4]^-$	58.80	54.86	3.94	58.81	0.01
5	$[KOAc]^0$	129.68	133.55	3.87	132.46	2.78
6	$[K(H_2O)]^+$	17.38	17.83	0.45	17.73	0.35
7	$[K(H_2O)_6]^+$	65.64	68.13	2.49	66.92	1.28
8	$[K(H_2O)_7]^+$	68.80	73.42	4.82	69.08	0.48
9	$[ZnOAc]^+$	424.79	451.13	26.34	436.58	11.79
10	$[Zn(OAc)_2]^0$	727.11	753.47	26.36	735.68	8.57
11	$[Zn(OAc)_3]^-$	941.46	957.75	16.29	944.16	2.70
12	$[Zn(OAc)_4]^{2-}$	1043.45	1045.59	2.14	1036.34	7.11
13	$[Zn(H_2O)]^{2+}$	100.95	95.82	5.13	96.15	4.80
14	$[Zn(H_2O)_6]^{2+}$	367.96	362.02	5.94	363.43	4.53
15	$[ZnOAc(H_2O)_4]^+$	563.55	559.42	4.13	561.39	2.16
16	$[ZnOAc(H_2O)_5]^+$	564.93	561.97	2.96	563.43	1.50
	Mean Error:			7.11		3.00
	Units:	**kcal/mol**	**kcal/mol**	**kcal/mol**	**kcal/mol**	**kcal/mol**

2. SUPPLEMENTARY FIGURES 1-13

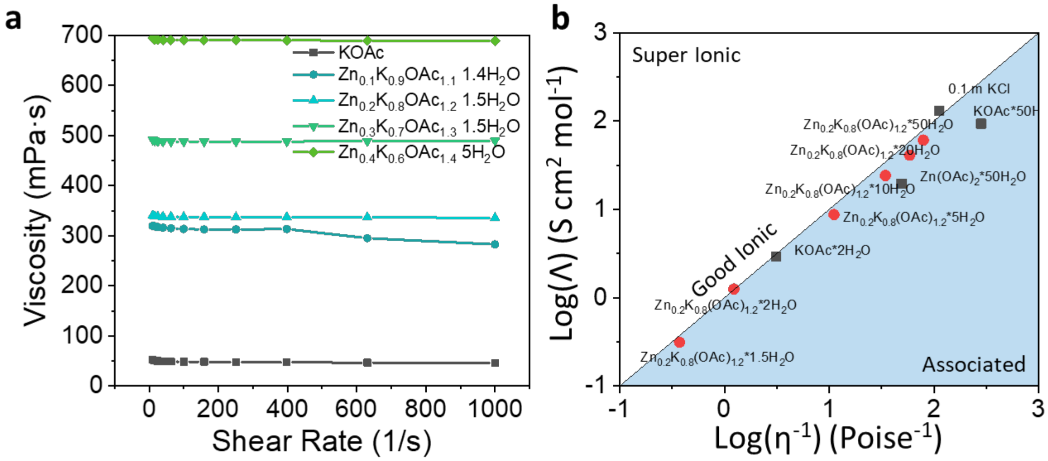

Figure S1. Physicochemical properties of the electrolyte. (a) Viscosity of the electrolytes $Zn_{(x)}K_{(1-x)}OAc_{(1+x)}$ nH_2O around the eutectic point. (b) Walden plot for the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes.[2]

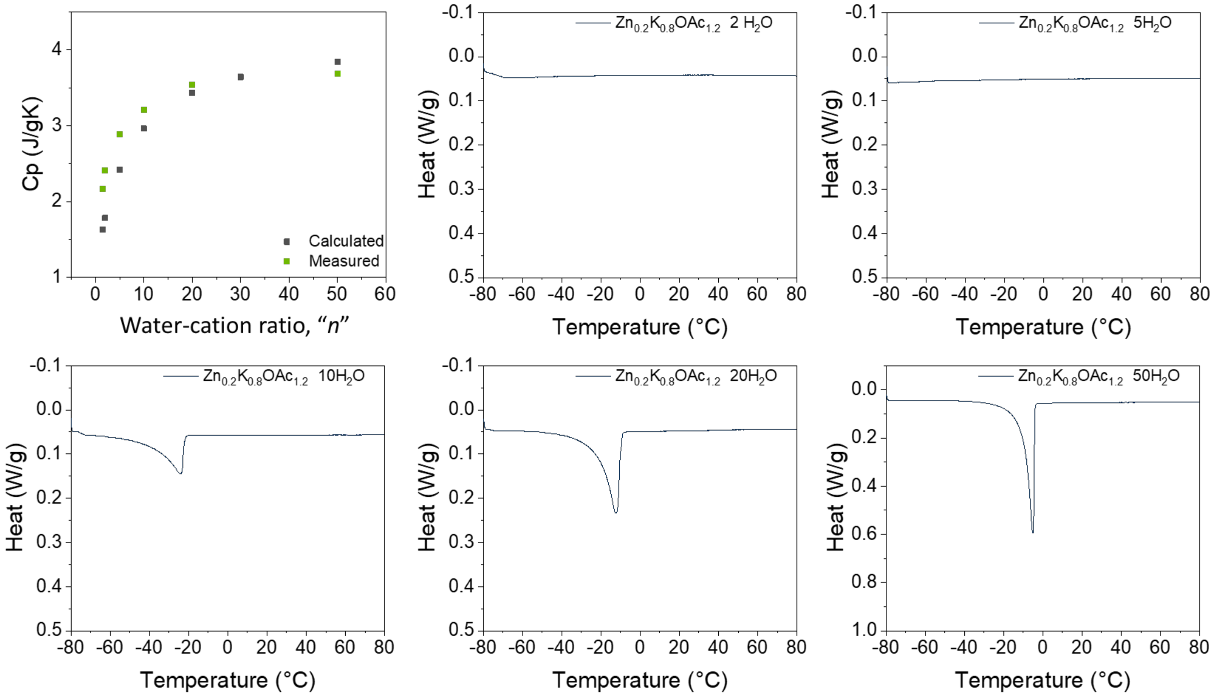

Figure S2. Thermal properties for the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes. (a) Shows the C_p as function of n. (b)-(f) shows the differential scanning calorimetry collected at 1°C/min from -80 to 80 for n=2, 5, 10, 20 and 50 respectively. The measured C_p values were extracted from the DSC results at 25°C. The calculated values were calculated using the C_p of the individual components in a linear combination. The main contribution for the C_p values comes from water (4.2 J/gK vs ~1 J/gK for the salts).

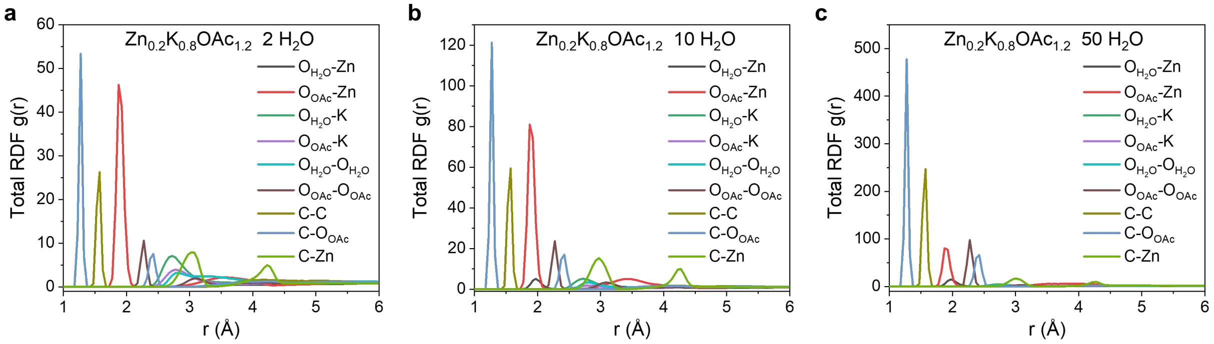

Figure S3. MD-derived total RDF main pair contributions for the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O with n=2 (a), 10 (b) and 50 (c)

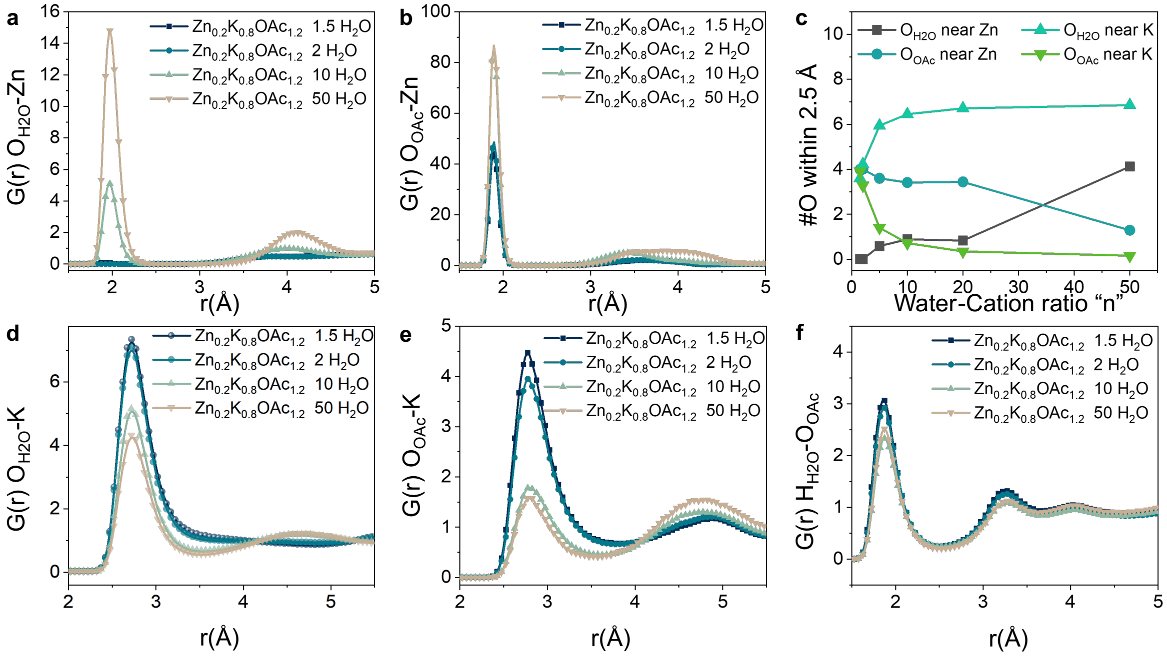

Figure S4. RDFs with the main X-O interactions as function of water-cation ratio "n" extracted from MD. (a) Zn-O_{H2O} (b) Zn-O_{OAc} (c) Extracted coordination composition for the cations within 2.5 A. (d) K-O_{H2O} (e)Zn-O_{OAc} (f) H_{H2O}-O_{OAc}

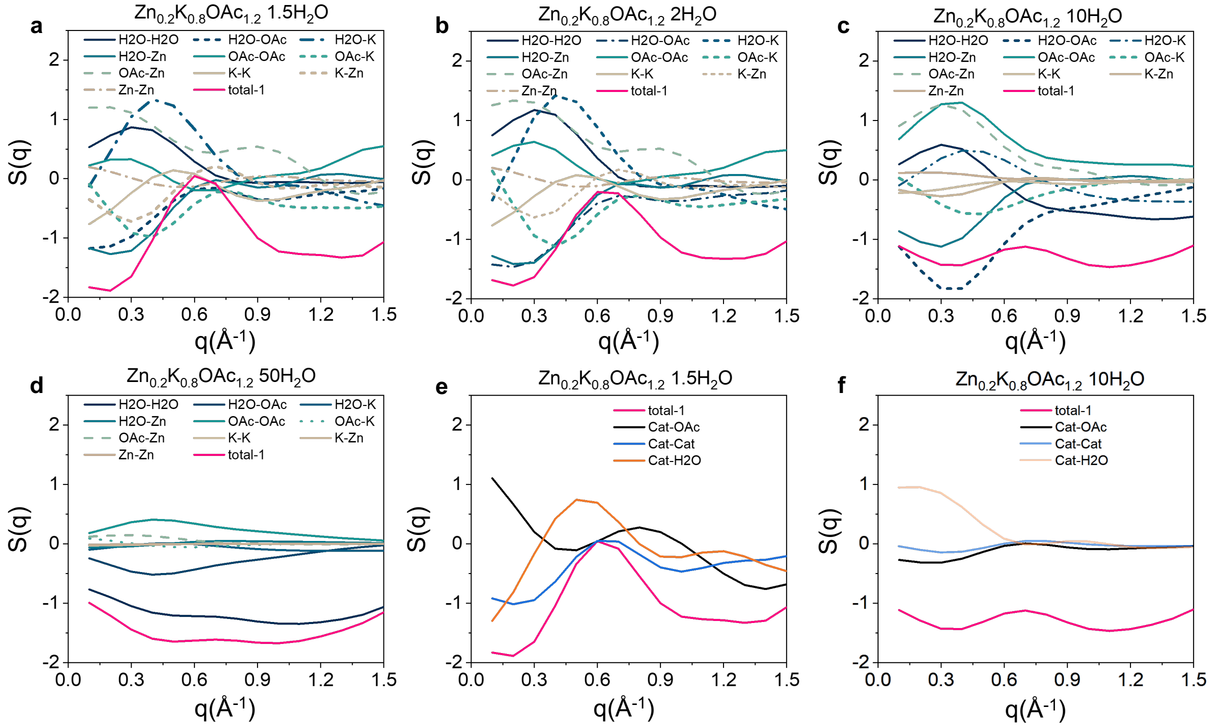

Figure S5. MD generated S(q) partials for the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O with n=1.5 (a), 2 (b), 10 (c), and 50 (d). Main interactions for the nanoscale segregation at n=1.5 (e), and 10 (f).

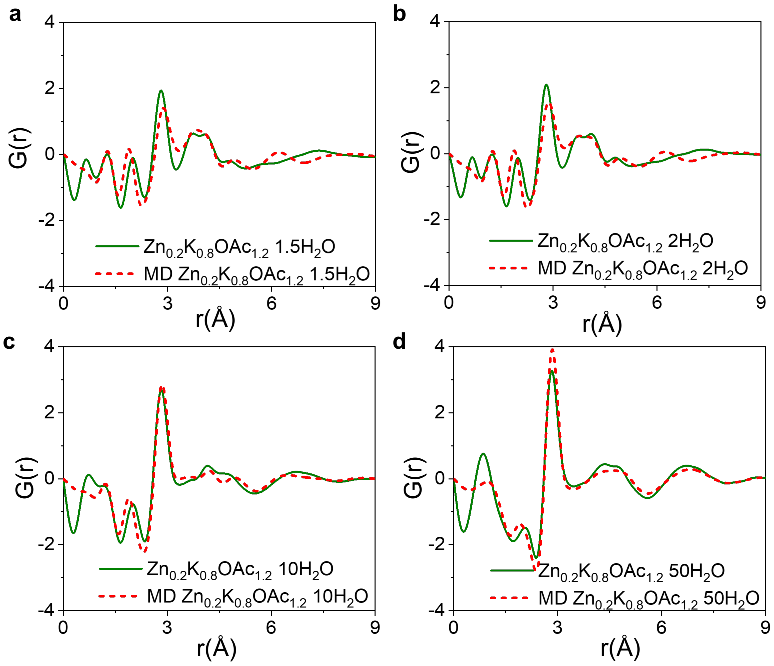

Figure S6. Comparison for the X-Ray scattering between MD and the experimental data for the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O (a)-(d) Show the PDF for n=1.5, 2, 10 and 50 respectively.

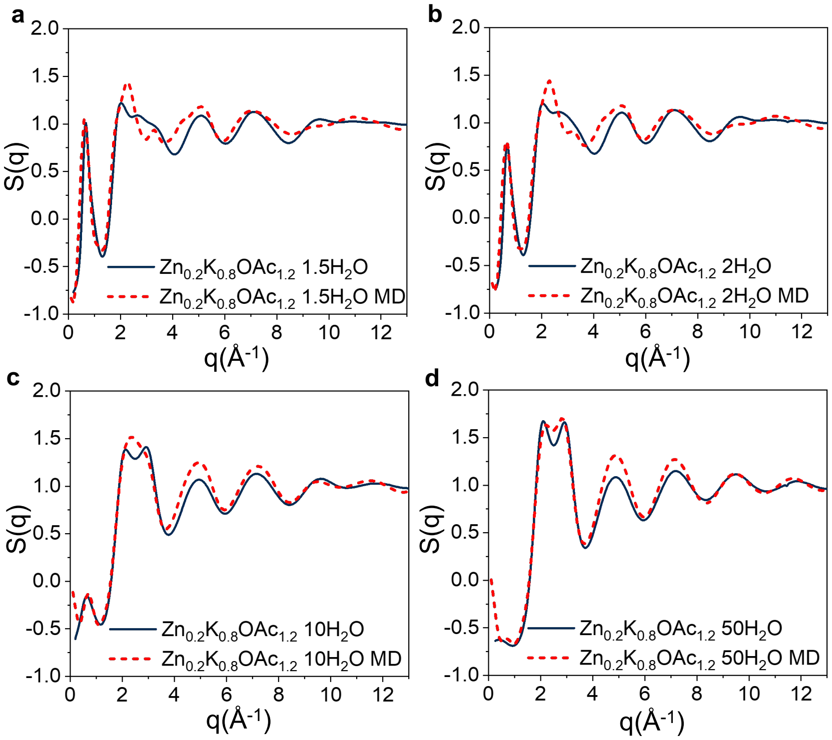

Figure S7. Comparison for the X-Ray scattering between MD and the experimental data for the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O (a)-(d) Show the S(q) for n=1.5, 2, 10 and 50 respectively.

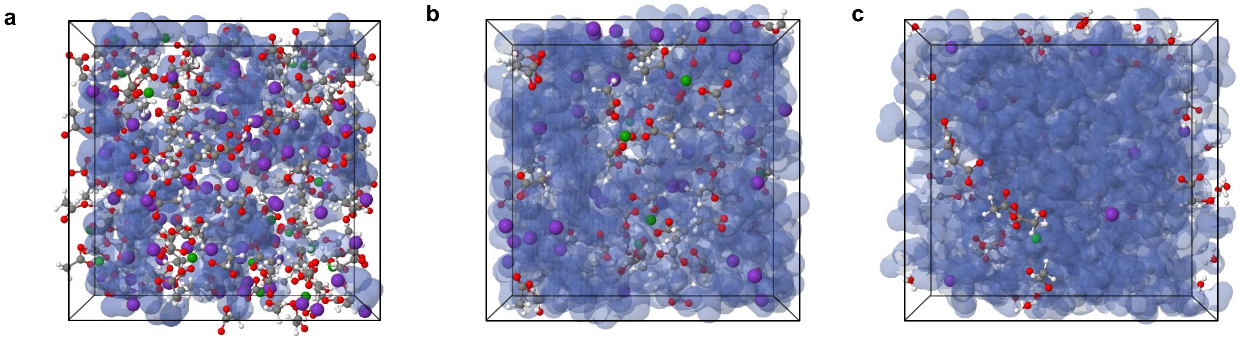

Figure S8. Water structure in the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes. (a)-(c) show the small simulation boxes with water domains (blue). Color scheme: Zn – green, K – purple, O – red, H – white and C – gray.

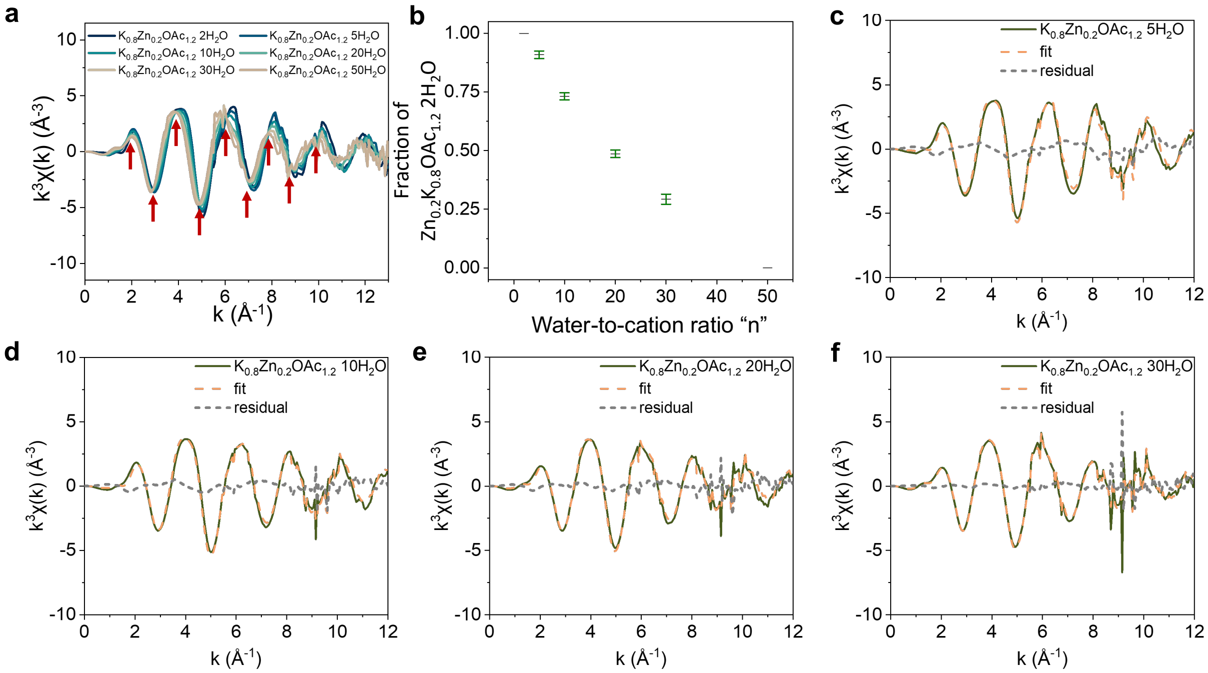

Figure S9. EXAFS fitting to linear combinations of the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O with n=2 and n=50. (a) Isosbestic points visualization (red arrows) from the k-space k^3 weighted for the electrolytes $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O with n= 2, 5, 10, 20, 30 and 50. (b) Linear combination fitting results. (c)-(f) Fitting in k-space k^3 weighted for n= 5, 10, 20 and 30 respectively.

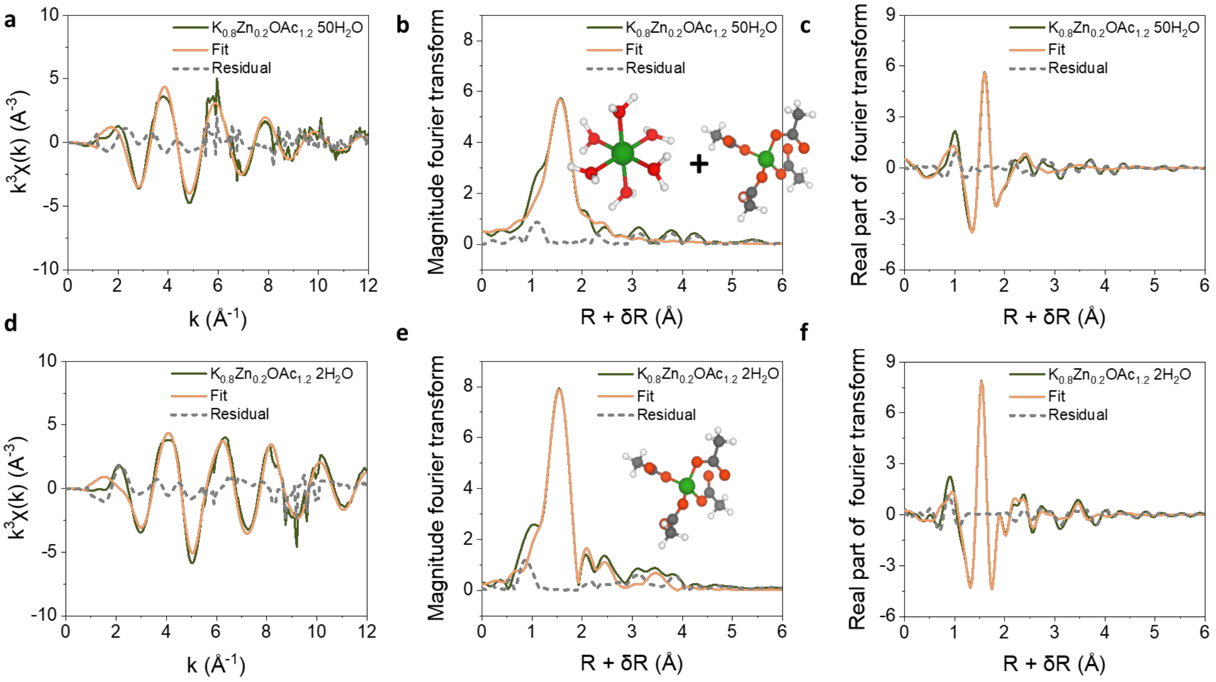

Figure S10. Fitting of the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes to the best DFT model. The fitting is represented in k-space, radial distance (magnitude) and radial distance (real part) with a k^3 weighing. (a)-(c) fitting for n=50 to a combination of x $Zn(H_2O)_6^{2+}$ octahedral and (1-x) $Zn(OAc)_4^{2-}$ tetrahedral models. R range 1.2-3 Å, k space 3-12 $Å^{-1}$. (d)-(f) fitting for n=2 to Zn-4(OAc) tetrahedral model. R range 1.2-4.5 Å, k space 3-12 $Å^{-1}$.

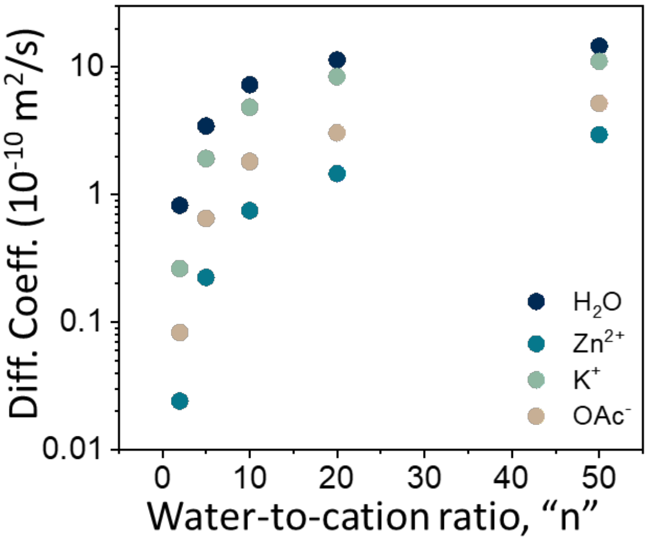

Figure S11. MD derived diffusion coefficients of the electrolyte components as a function of water-to-cation "n" ratio for the electrolyte series $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O

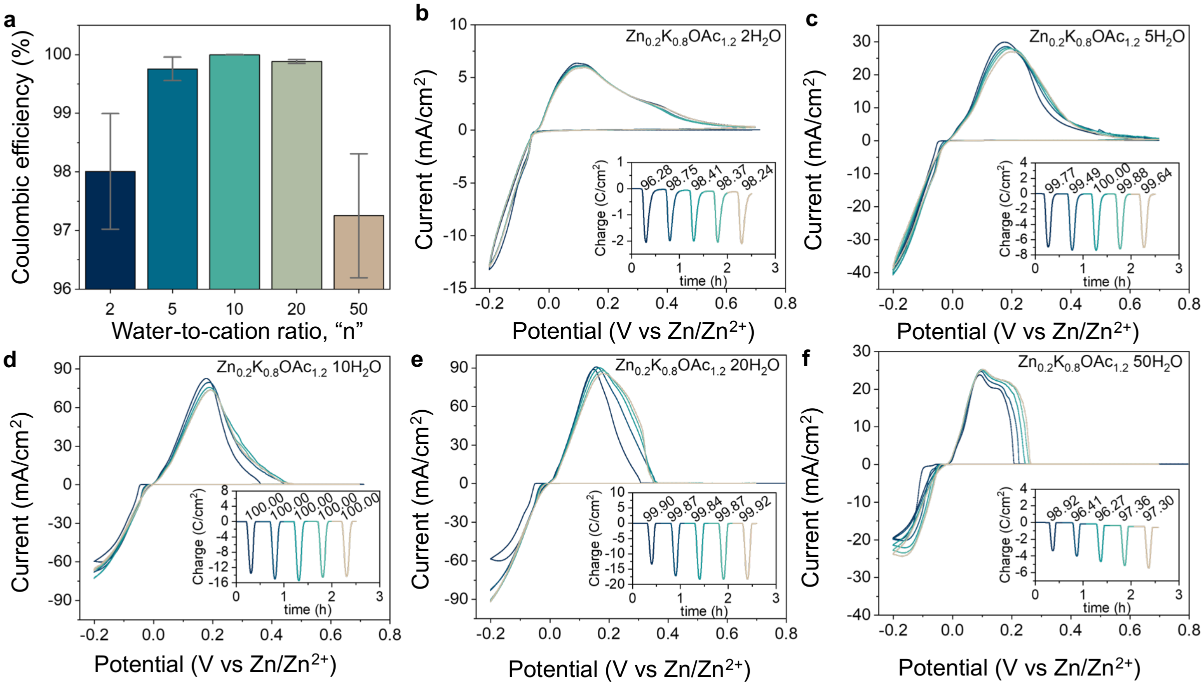

Figure S12 Cyclic voltammetry profiles collected at 1 mV/s on Au disk electrodes in Zn-K acetate electrolytes. (a) Averaged Coulombic efficiency as function of water-to-cation ratio "n" for the electrolyte series $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O. CV profiles of Zn plating/stripping for the first 5 cycles, Insert: Charge vs time with Coulombic efficiencies per cycle collected in (b) $Zn_{0.2}K_{0.8}OAc_{1.2}$ $2H_2O$, (c) $Zn_{0.2}K_{0.8}OAc_{1.2}$ $5H_2O$, (d) $Zn_{0.2}K_{0.8}OAc_{1.2}$ $10H_2O$, (e) $Zn_{0.2}K_{0.8}OAc_{1.2}$ $20H_2O$, (f) $Zn_{0.2}K_{0.8}OAc_{1.2}$ 50 H_2O.

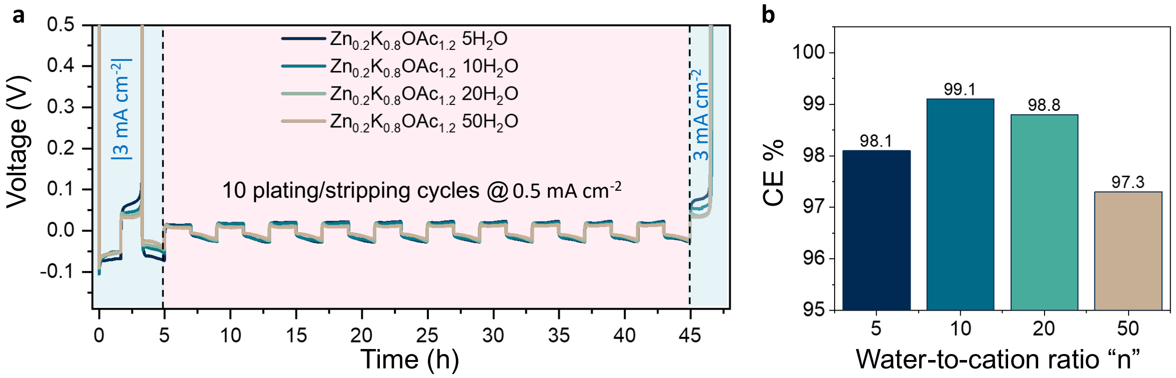

Figure S13. Aurbach coulombic efficiency test collected in different electrolytes. (a) Respective voltage profiles. (b) Calculated coulombic efficiency (CE) as a function of electrolyte composition.

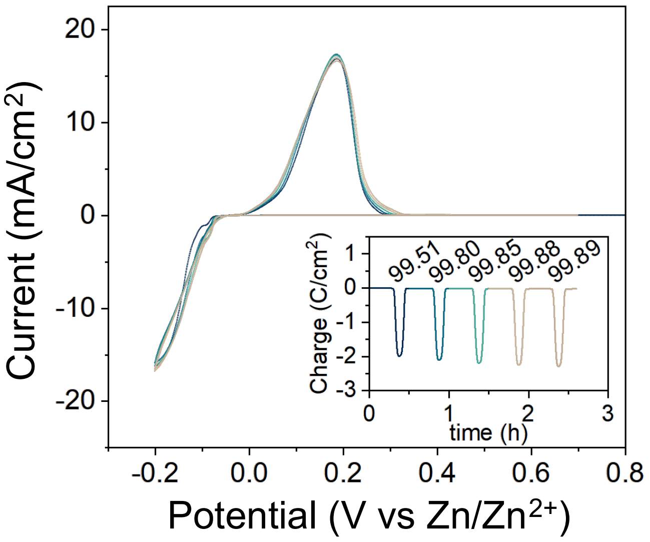

Figure S14. Cyclic voltammetry profiles collected at -5°C at 1 mV/s on Au disk electrodes in $Zn_{0.2}K_{0.8}OAc_{1.2}$ $10H_2O$. Insert: Charge vs time with Coulombic efficiencies per cycle.

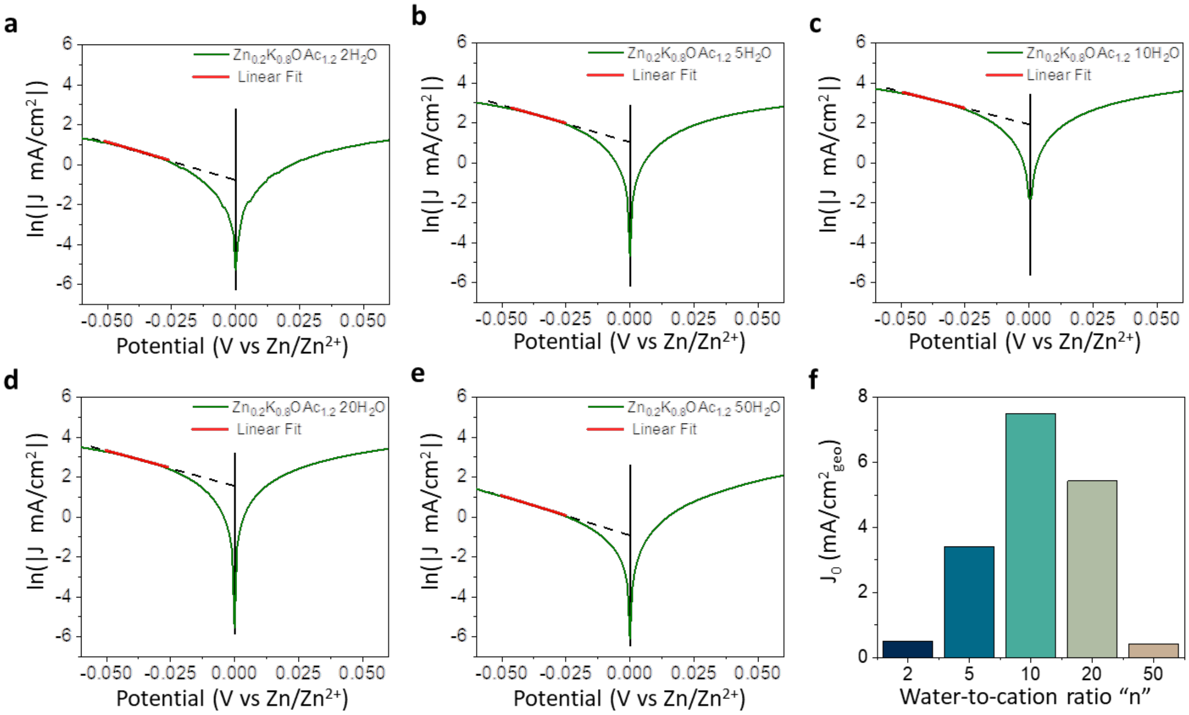

Figure S15. Tafel slopes for the $Zn_{0.2}K_{0.8}OAc_{1.2}$ nH_2O electrolytes (green) and the fitting window (red). (a)-(e) Shows the results for n= 50, 20, 10, 5 and 2 respectively. (f) Shows the exchange current values extracted

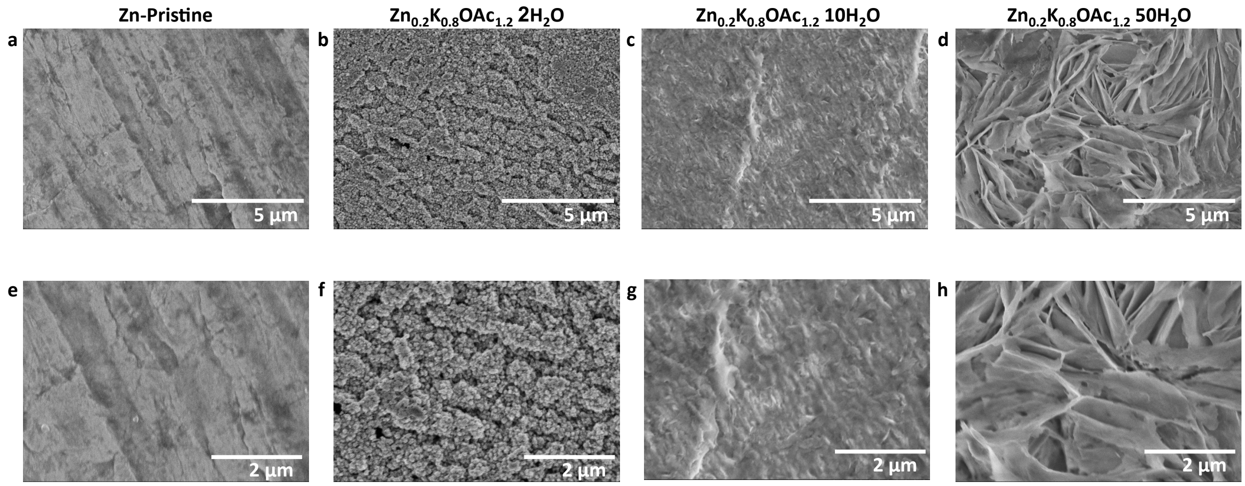

Figure S16. The SEM images collected at different magnifications of the pristine Zn foil (a and e) and Zn electrodes after 10 galvanostatic cycles (1 mA/cm^2, Zn-Zn symmetric cells configuration) in different electrolytes: $Zn_{0.2}K_{0.8}OAc_{1.2}$ $2H_2O$, (b and e) (d) $Zn_{0.2}K_{0.8}OAc_{1.2}$ $10H_2O$ (c and g) and $Zn_{0.2}K_{0.8}OAc_{1.2}$ 50 H_2O (d and h).

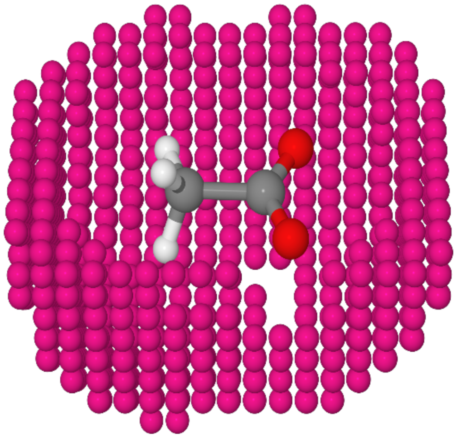

Figure S17. Grid points (pink) with unit charge used to fit polarizabilities for acetate.

3. SUPPLEMENTARY TEXT

a. Molecular dynamics simulation methodology and the force field development

All molecular dynamics (MD) simulations were performed using a locally modified version of Tinker HP v1.2 software,[3] which allows for saving of stress tensor every 4 fs that was used to compute viscosity and the finite-size correction to diffusivities and conductivity following the previously described procedure for extracting transport properties.[4] We make use of the water, Zn^{2+}, and K^{+} parameters of the AMOEBA09 polarizable force field *as is*.[5-6] Initial parameters for acetate were taken from literature[7] though we refit atomic polarizabilities and made some specific adjustments to the mixed vdW pair interactions. We call this force field iteration 1 (FF1). All parameters are appended to the end of this document in Tinker format. While these parameters performed reasonably well in reproducing binding energies relative to counterpoise-corrected ωB97X-D/6-311++G(3df,3pd) DFT calculations (see **Table S4**), the smaller Zn-OAc clusters were strongly over binding. To correct this, we refit the multipoles taking care to zero the quadrupole values for the carboxylate atoms (COO) as discussed in literature to better balance mono- vs bidentate binding.[8] We make an additional adjustment to the vdW pair interactions in this case as well. Collectively, this new force field is called force field iteration 2 (FF2). In **Table S4**, we show that the problematic overestimation of binding energies for the $Zn(OAc)_n$, where n=1..4 clusters is somewhat alleviated. Despite the improvement in binding energies, MD simulations using FF1 better reproduces the experimental conductivity across the concentration range while MD simulations using FF2 overestimates conductivities. Consequently, the presentation of results and their discussion will focus on MD simulations using the FF1 parameter set unless otherwise noted. The DFT calculations were performed using Gaussian 16 rev C.01 in combination with the Atomic Simulation Environment and Openbabel for calculation preparation and coordinate generation.[9-11]

b. Detailed discussion of molecular dynamics calculations: simulation workflow

Initial configurations were generated using a random seed in Packmol[12] for several water:$Zn_{0.2}K_{0.8}OAc_{1.2}$ ratios (50:1, 20:1, 10:1, 5:1, 2:1, and 1.5:1). For the systems with water:salt ratios of 50:1, 20:1, and 10:1, three unique configurations (replicates) for each ratio were generated with a box length of ~40 Å based on experimental densities. Each of the 50:1 and 20:1 systems have 2,000 waters and the 10:1 systems each have 1,600 waters. For the systems with 10:1, 5:1, 2:1, and 1.5:1, three replicates were initialized based on the experimental density but with a box length of ~25 Å. These systems had 400 (10:1), 350 (5:1), 200 (2:1), and 150 (1.5:1) waters each. After preparation, geometries were initially minimized with polarization turned off to remove close contacts and stabilize the system for initial MD. Equilibration was performed identically for all concentrations and all replicates, sequentially stepping through each of the following:

1) 8 ns at 363.15 K (NVT) [2 fs timestep, RESPA integrator, Bussi thermostat]
2) 8 ns at 333.15 K (NVT) [2 fs timestep, RESPA integrator, Bussi thermostat]
3) 8 ns at 293.15 K (NVT) [2 fs timestep, RESPA integrator, Bussi thermostat]
4) 8 ns at 293.15 K (NPT) [1 fs timestep, Beeman integrator, Berendsen barostat, Bussi thermostat] (measure: average density over last 4 ns, rescale box)
5) 8-12 ns at 293.15 K (NVT) [2 fs timestep, RESPA integrator, Bussi thermostat]

For all concentrations and replicates, 56-60 ns of additional simulation beyond this equilibration period were performed and passed to analysis. Timestep, thermostat, and integrator are identical to step #5 above. In all calculations, 10 Å cutoffs were used for non-bonded interactions with PME grids of 42x42x42 and 28x28x28 for the large and small size cells, respectively. A long-range vdW correction term is considered as well. Center of mass drift was removed at every timestep.

c. Force field iteration 1 parameters:

```
# atom types

atom          1    1    O     "AMOEBA Water O"                8    15.995    2
atom          2    2    H     "AMOEBA Water H"                1     1.008    1
atom          8    8    K+    "Potassium Ion K+"             19    39.098    0
atom         13   13    Zn+   "Zinc Ion Zn+2"                30    65.390    0
atom        500  500    C     "Acetate CH3"                   6    12.011    4
atom        501  501    H     "Acetate H3C"                   1     1.008    1
atom        502  502    C     "Acetate COO"                   6    12.011    3
atom        503  503    O     "Acetate OOC"                   8    15.999    1



# amoeba09 water, as is
vdw           1               3.4050     0.1100
vdw           2               2.6550     0.0135       0.910
bond          1    2          556.85     0.9572
angle         2    1    2      48.70     108.50
ureybrad      2    1    2      -7.60     1.5326
multipole     1   -2   -2              -0.51966
                                        0.00000     0.00000    0.14279
                                        0.37928
                                        0.00000    -0.41809
                                        0.00000     0.00000    0.03881
multipole     2    1    2               0.25983
                                       -0.03859     0.00000   -0.05818
                                       -0.03673
                                        0.00000    -0.10739
                                       -0.00203     0.00000    0.14412
polarize      1           0.837      0.390        2
polarize      2           0.496      0.390        1
```

```
# amoeba09 K/Zn, as is

vdw           8               3.6800     0.3500

vdw          13               2.6800     0.2220

multipole     8    0    0               1.00000

                                        0.00000    0.00000    0.00000

                                        0.00000

                                        0.00000    0.00000

                                        0.00000    0.00000    0.00000

multipole    13    0    0               2.00000

                                        0.00000    0.00000    0.00000

                                        0.00000

                                        0.00000    0.00000

                                        0.00000    0.00000    0.00000

polarize      8          0.7800     0.3900

polarize     13          0.2600     0.2096
```

```
# force field iteration 1 acetate, vdW, charge-dipole-quadrupole, and bonded terms
# from https://aip.scitation.org/doi/10.1063/1.4985921
vdw         500               3.8200     0.1010
vdw         501               2.9800     0.0240     0.9400
vdw         502               3.8200     0.1060
vdw         503               3.5500     0.0950
bond        500  501          380.96     1.0977
bond        500  502          345.25     1.5610
bond        502  503          631.79     1.2640
angle       501  500  501      47.36     109.28
angle       501  500  502      41.54     107.90
angle       500  502  503      70.71     114.97
angle       503  502  503      68.38     134.00
strbnd     501   500   502   11.50   11.50
strbnd     500   502   503   18.70   18.70
strbnd     503   502   503   18.70   18.70
opbend     500   502   0   0   52.4446
opbend     503   502   0   0   56.7610
torsion    501   500   502   503   -0.154 0.0 1   0.044 180.0 2  -0.086 0.0 3
multipole   500  502  503              -0.27876
                                        0.00000    0.00000    0.03145
                                       -0.02428
                                        0.00000   -0.02428
                                        0.00000    0.00000    0.04856
multipole   501  500  502               0.01209
                                        0.01717    0.00000   -0.16145
                                        0.07658
                                        0.00000    0.12458
                                       -0.04982    0.00000   -0.20116
multipole   502 -503 -503               0.99851
                                        0.00000    0.00000    0.09895
                                        0.00000
                                        0.00000    0.00000
                                        0.00000    0.00000    0.00000
```

```
multipole   503  502  503              -0.87801
                                        0.00000    0.00000   -0.03127
                                        0.00000
                                        0.00000    0.00000
                                        0.00000    0.00000    0.00000
# these are re-fitted to wB97XD/6-311++G(3df,3pd), they are NOT from the above paper
polarize    500          1.2000     0.3900      501    502
polarize    501          0.3500     0.3900      500
polarize    502          1.2000     0.3900      500    503
polarize    503          1.5500     0.3900      502
# specific mixing
vdwpr  2  503  3.1967  0.02848  # improved Eint with water monomer through tetramer
vdwpr  8  503  3.6900  0.1659   # slight improvement to geometry, no real improvement
on energy
```

d. Acetate parameters in force field iteration 2:

```
# bonded, vdW, polarization unchanged; electrostatics refit using Stone’s DMA
# however, I do still zero the quadrupole for COO atoms, as discussed in
# https://aip.scitation.org/doi/10.1063/1.4985921
multipole     500  502  503            -0.13285
                                        0.01502    0.00000    0.15811
                                        0.15623
                                        0.00000   -0.00422
                                        0.00401    0.00000   -0.15201
multipole     501  500  502             0.06148
                                        0.11557    0.00000    0.19263
                                       -0.03074
                                        0.00000   -0.34488
                                        0.28710    0.00000    0.37562
multipole     502 -503 -503             0.43765
                                       -0.00346    0.00000    0.00221
                                        0.00000
                                        0.00000    0.00000
```

```
                                        0.00000    0.00000    0.00000
multipole     503  502  503            -0.74462
                                        0.05832    0.00000    0.04990
                                        0.00000
                                        0.00000    0.00000
                                        0.00000    0.00000    0.00000
# specific mixing
vdwpr  2  503  3.1321  0.02848
vdwpr  8  503  3.6900  0.1659
```

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