

## SUPPLEMENTARY MATERIAL

### “Molecular Dynamics Study of Perchloric Acid Using the Extended Madrid-2019 Force Field.”

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The Supplementary Material for the publication ‘Molecular Dynamics Study of Perchloric Acid Using the Extended Madrid-2019 Force Field’ contains the compilation of the numerical (raw data) and graphical information of the simulation results of perchloride acid solutions considered in the main body of this work for the following properties:

- Simulation results for the density ( $\rho^{\text{sim}}$ ) as a function of the molality ( $m$ ) and the temperatures 283.15, 298.15, and 323.15 K. The experimental data ( $\rho^{\text{exp}}$ ) were obtained from Ref. [1].
- Density as a function of temperature for aqueous solutions of perchloric acid ( $\text{HClO}_4$ ) at 0.98 ( $m$ ), 0.69 ( $m$ ), 0.49 ( $m$ ), and 0.30 ( $m$ ) at 1 bar.
- Variation of  $\Delta$  as a function of  $m$  for perchloric acid solutions.
- Self-diffusion coefficients of water ( $\text{H}_2\text{O}$ ) and perchloric ion ( $\text{ClO}_4^-$ ) as a function of molality at 298.15 K and 1 bar.
- Shear viscosity as a function of molality for aqueous solutions of perchloric acid ( $\text{HClO}_4$ ) at 298.15 K and 1 bar compared with experimental data obtained from Ref. [1].

## I. RAW DATA

### A. Bulk densities

Table S I. Comparison between simulation results and experimental data for the bulk density for perchloric acid solutions at 283.15 K, 298.15 K, and 323.15 K. Experimental data were obtained from Ref. [1]. The relative percentage deviation is given by  $\text{dev.}(\%) = 100 \times |\rho^{\text{exp}} - \rho^{\text{sim}}| / \rho^{\text{exp}}$ . Units: mol/kg for  $m$  and  $\text{kg/m}^3$  for density,  $\rho$ .

283.15 K				298.15 K				323.15 K			
$m$	$\rho^{\text{exp}}$	$\rho^{\text{sim}}$	dev.(%)	$m$	$\rho^{\text{exp}}$	$\rho^{\text{sim}}$	dev.(%)	$m$	$\rho^{\text{exp}}$	$\rho^{\text{sim}}$	dev.(%)
0.00	1000.00	1001.16	0.12	0.00	997.10	997.30	0.02	0.00	988.00	988.33	0.03
0.98	1054.05	1058.20	0.39	0.98	1049.41	1052.63	0.31	0.98	1037.69	1040.04	0.23
1.93	1103.53	1108.53	0.45	1.93	1095.94	1100.83	0.45	1.93	1081.80	1085.56	0.35
3.74	1187.25	1192.90	0.48	3.74	1177.90	1182.35	0.38	3.74	1160.29	1163.27	0.26
5.42	1257.23	1262.06	0.38	5.42	1245.63	1247.43	0.14	5.42	1226.14	1227.79	0.13
6.22	1287.30	1292.13	0.38	6.22	1275.70	1278.74	0.24	6.22	1254.99	1255.70	0.06
7.00	1315.72	1319.60	0.29	7.00	1303.20	1305.61	0.18	7.00	1282.06	1281.85	0.02
8.48	1366.94	1369.31	0.17	8.48	1353.39	1353.90	0.04	8.48	1330.20	1328.94	0.09

Table S II. Density of perchloric acid solutions as a function of temperature and molalities: 0.30  $m$ , 0.49  $m$ , 0.69  $m$ , and 0.98  $m$ . Units: mol/kg for  $m$ , K for  $T$ , and  $\text{kg/m}^3$  for  $\rho$ .

0.30 m		0.49 m		0.69 m		0.98 m	
$T$	$\rho^{\text{sim}}$	$T$	$\rho^{\text{sim}}$	$T$	$\rho^{\text{sim}}$	$T$	$\rho^{\text{sim}}$
240	1010.23	240	1025.04	240	1039.39	230	1055.97
245	1013.39	245	1027.75	245	1041.51	235	1058.30
250	1015.80	250	1029.68	250	1043.03	240	1060.20
255	1017.52	255	1031.05	255	1044.07	245	1061.33
260	1018.66	260	1031.84	260	1044.34	250	1062.23
265	1019.52	265	1032.11	265	1044.37	255	1062.54
270	1019.65	270	1032.11	270	1044.12	260	1062.53
275	1019.50	275	1031.66	275	1043.43	265	1062.06
280	1019.14	280	1030.94	280	1042.44	270	1061.44
285	1018.29	285	1029.91	285	1041.27	275	1060.43
290	1017.29	290	1028.64	290	1039.79	280	1059.15
						285	1057.63
						290	1055.87

Table S III.  $\Delta$  of TMD for different molalities. Units: mol/kg for  $m$  and K for  $\Delta$ .

$m$	$\Delta$
0.30	-6.79
0.49	-10.84
0.69	-14.41
0.98	-20.38

### B. Self-Diffusion Coefficient

Table S IV. Simulation results for self-diffusion coefficient variation with molality for water,  $D_{H_2O}$ , and perchlorate anion,  $D_{ClO_4^-}$ . Units in mol/kg for  $m$  and  $\text{cm}^2/\text{s}$  for self-diffusion coefficient  $D_i$ .

$m$	$D_{H_2O}$	$D_{ClO_4^-}$
0.00	2.300	1.412*
0.98	2.276	1.316
3.74	1.939	1.035
5.42	1.591	0.815
8.48	1.081	0.545

\* Denotes linear interpolation from simulation data.

### C. Shear viscosity

Table S V. Comparison between simulation results and experimental data for shear viscosity variation with molality for  $\text{HClO}_4$ . Experimental data were obtained from Ref.[1]. Units in mol/kg for  $m$  and  $\text{mPa}\cdot\text{s}$  for shear viscosity  $\eta$ .

$m$	$\eta^{sim}$
0.00	0.85
0.98	0.91
3.74	1.12
5.42	1.24

## II. FIGURES

### A. Bulk densities

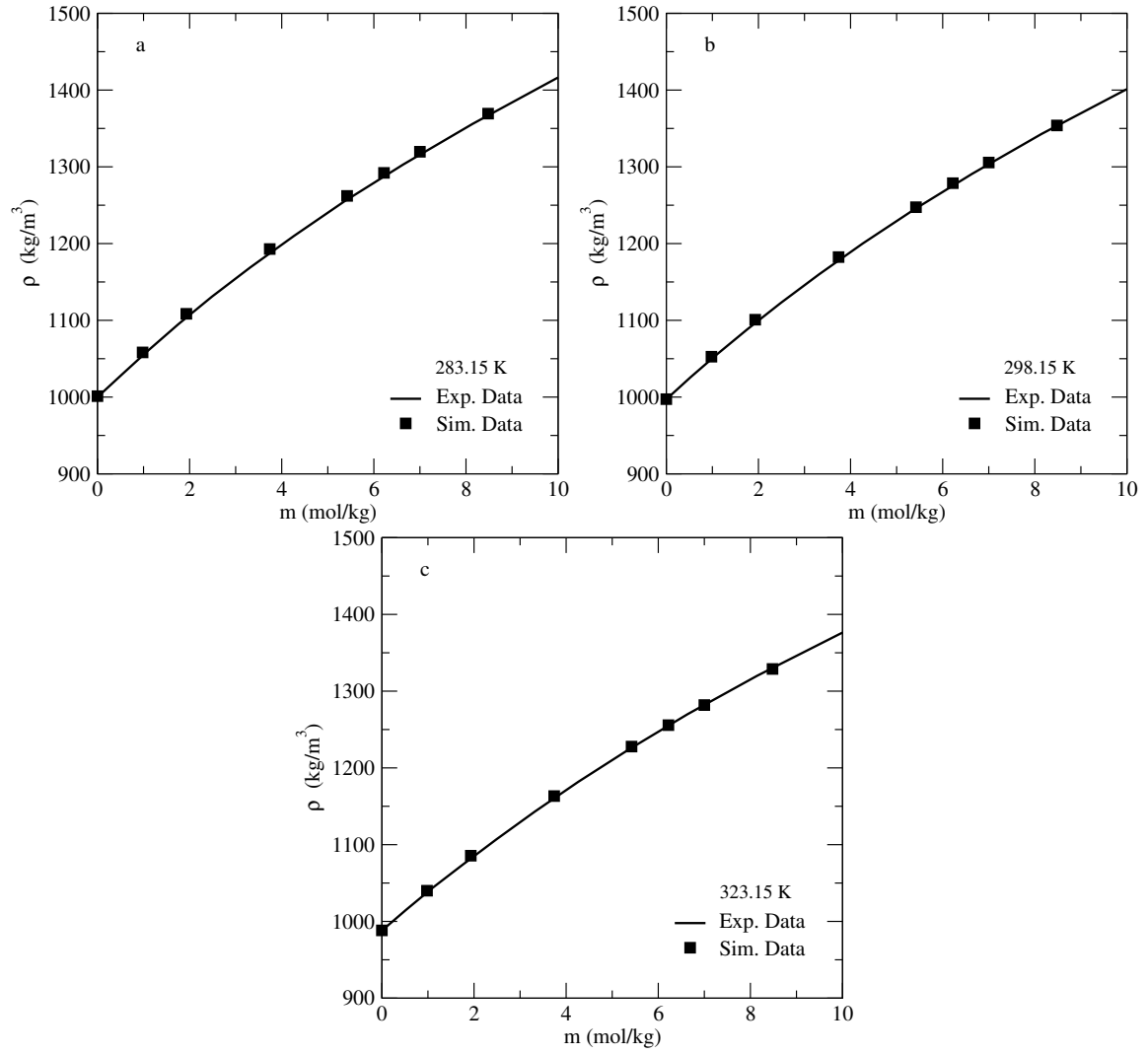


Fig. S 1. Density as a function of molality for aqueous HClO<sub>4</sub> solutions at 283.15 K (a), 298.15 K (b), and 323.15 K (c). MD results: black squares; experimental data: continuous lines (Ref. [1]).

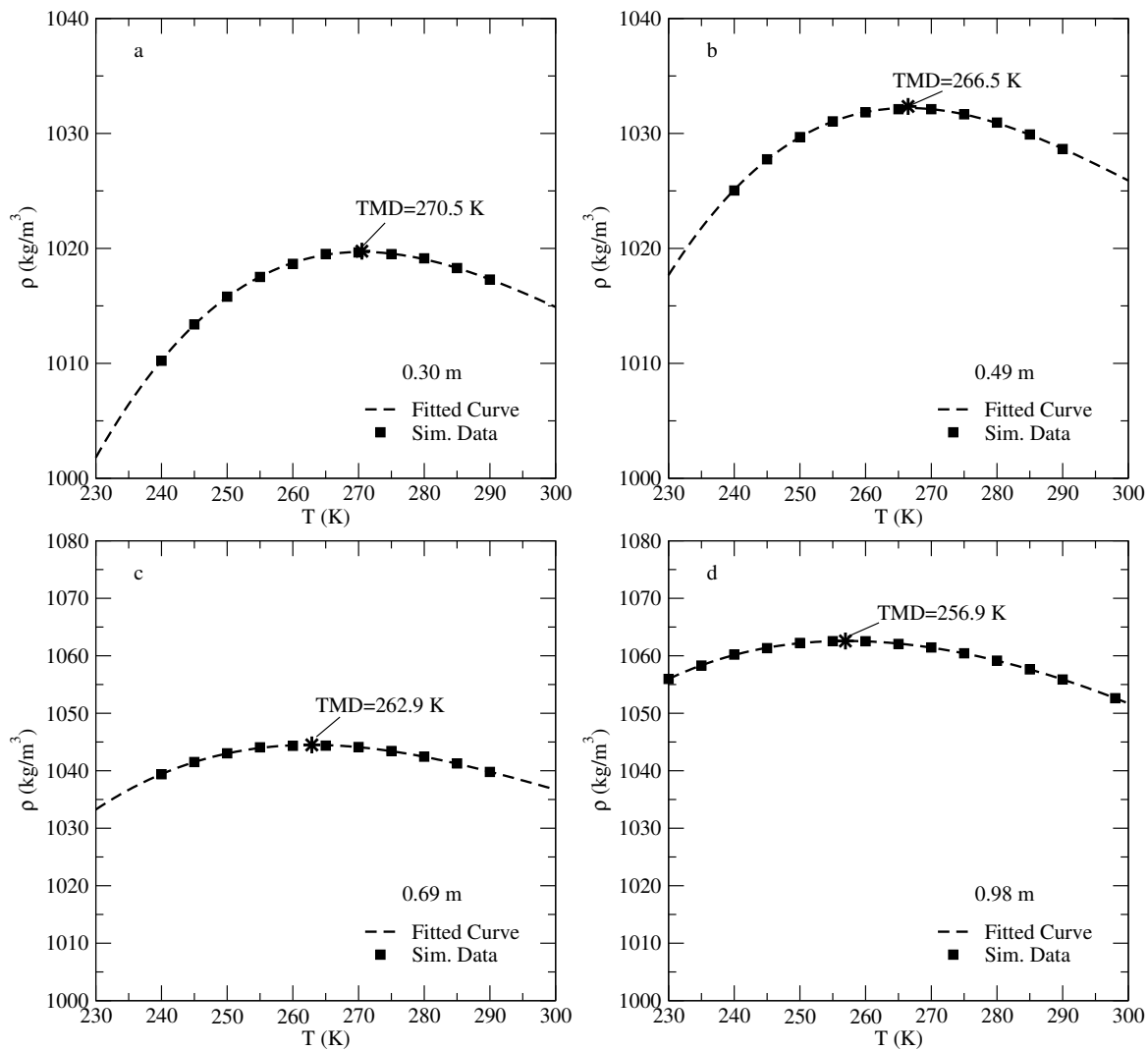


Fig. S 2. Density as a function of temperature at 0.30 m (a), 0.49 m (b), 0.69 m (c), 0.98 m (d) molalities.

### B. Shear viscosity

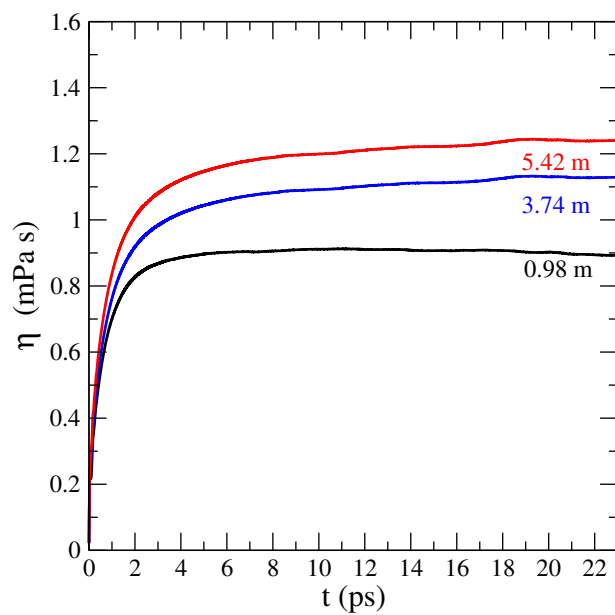


Fig. S 3. Running viscosity as a function of correlation time at 298.15 K and 1 bar.

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- [1] L. H. Brickwedde, "Properties of aqueous solutions of perchloric acid," *J. Res. Nat. Bur. Stand*, vol. 42, pp. 309–329, 1949.