Force Field Parameterization of Metal Ions From Statistical Learning Techniques - SUPPORTING INFORMATION

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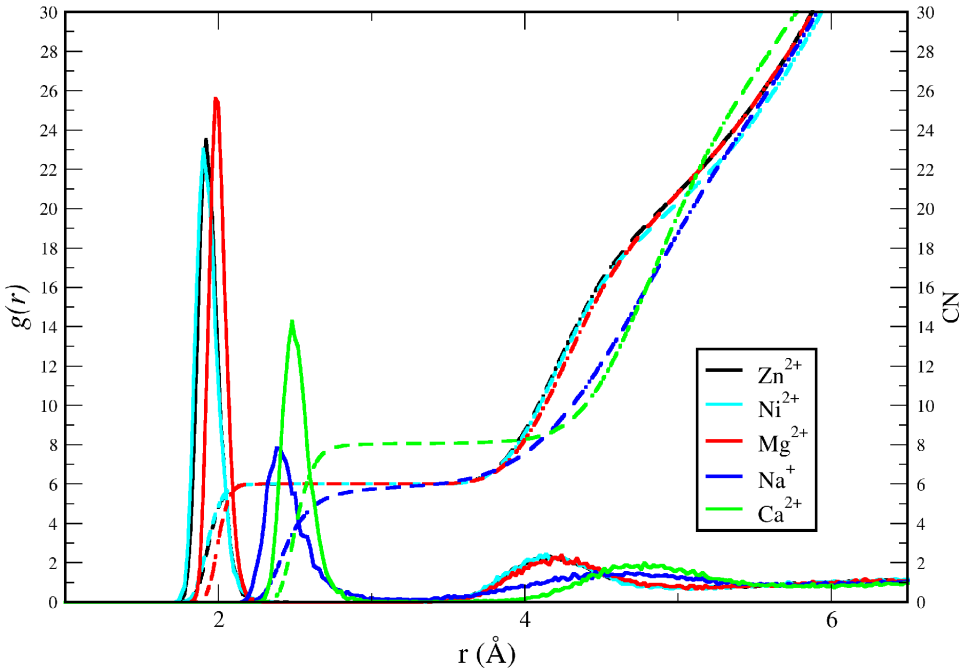

Figure S1: Computed radial distribution functions (rdf, solid lines) and running integration number (dashed lines) for the metal ion-water oxygens interaction in Molecular Dynamics simulations (NVT ensemble, room temperature) using Merz[1] (Zn^{2+}), Aqvist[2] (Mg^{2+}, Na^{+}) and Li et al.[3] (Ni^{2+}, Ca^{2+}) force fields.

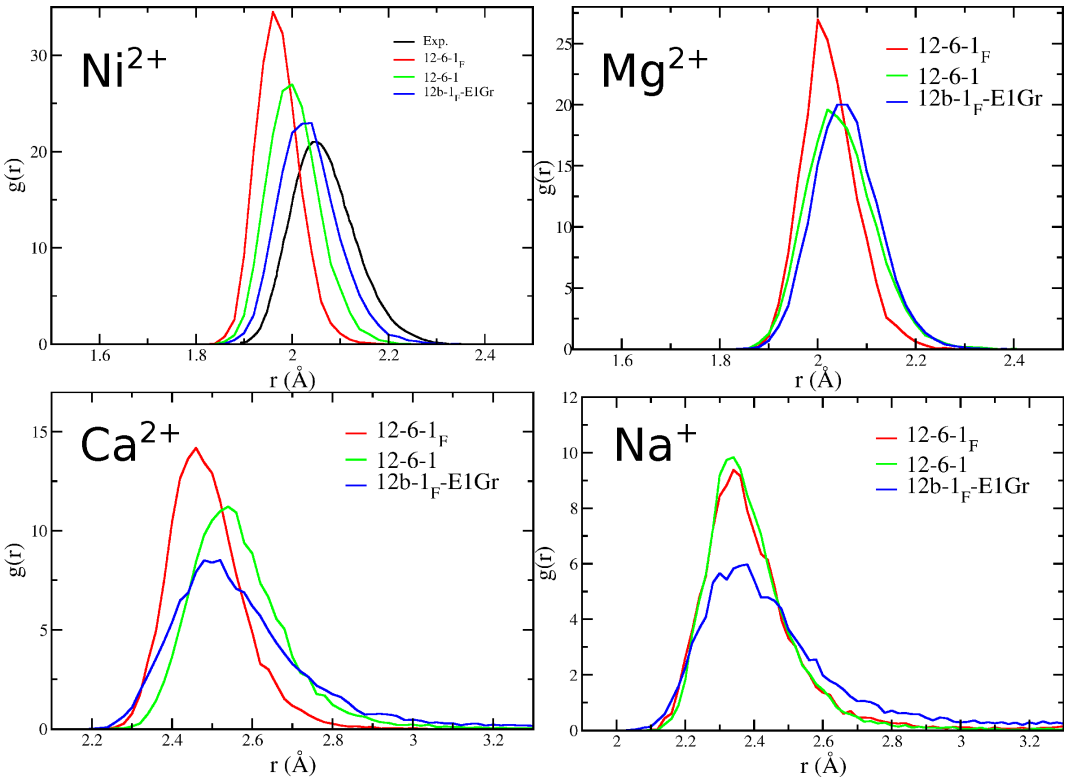

Figure S2: Computed radial distribution function between Ni^{2+}, Mg^{2+}, Ca^{2+}, Na^{+} and water oxygens, using the 12-6-1_F (red line), 12-6-1 (green) and 12b-1-E1Gr (blue) models. In the case of Ni^{2+}, also the experimental distribution (black line) is shown.

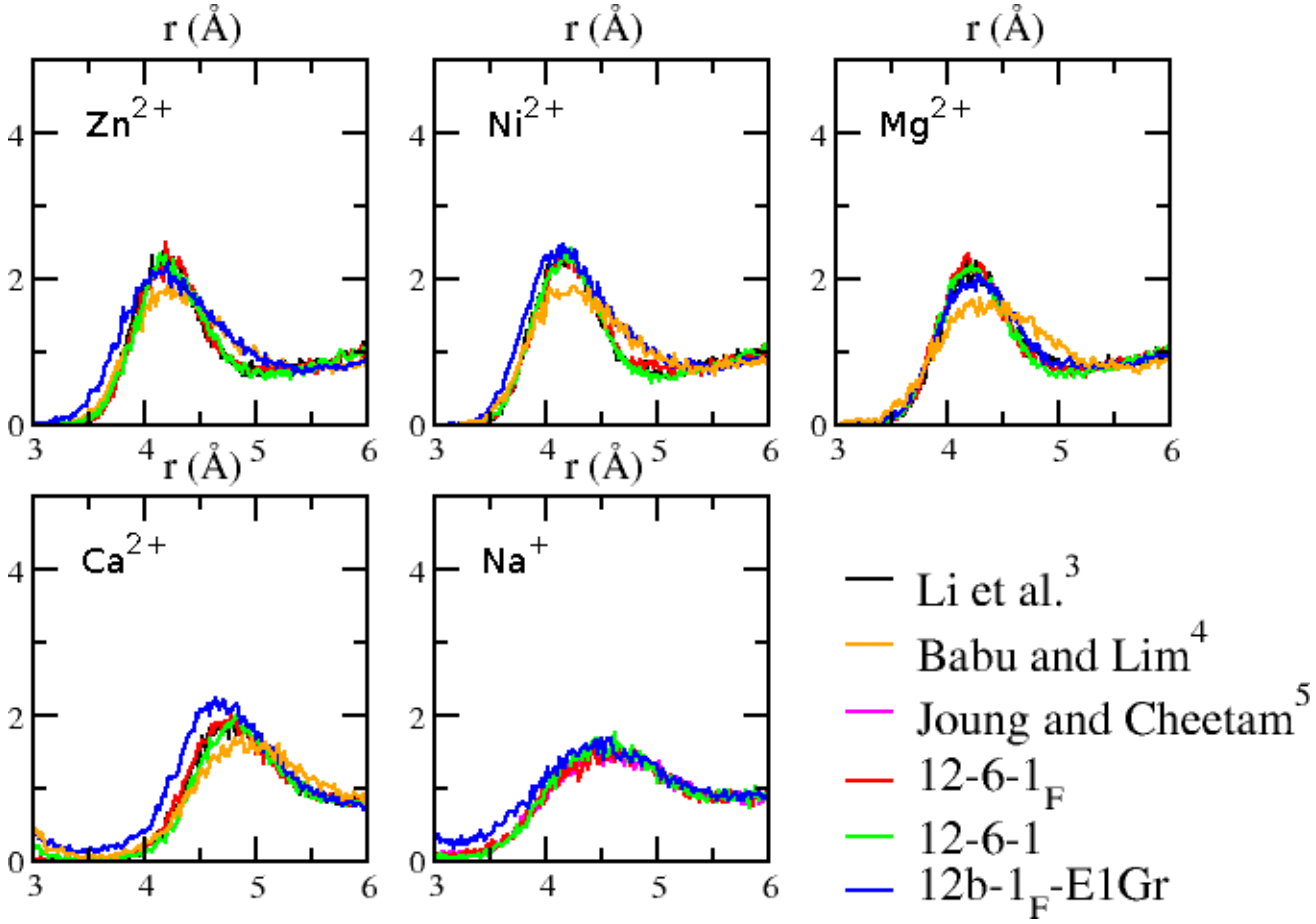

Figure S3: Second peak from radial distribution functions for the metal ion-water oxygens interaction in Molecular Dynamics simulations using the Li[3] (black line, Zn^{2+}, Ni^{2+}, Mg^{2+}, Ca^{2+}), Babu and Lim[4] (orange, Zn^{2+}, Ni^{2+}, Mg^{2+}, Ca^{2+}), Joung and Cheatham[5] (magenta, Na^{+}), 12-6-1_F (red), 12-6-1 (green) and 12b-1_F-E1Gr (blue) models.

Table S1: Metal ions LRR-DE optimized parameters for the 12-6-1_F model.

	σ (Å)	ϵ (kJ/mol)
Zn^{2+}	0.2339341	0.028551
Ni^{2+}	0.1145527	744.7884
Mg^{2+}	0.1939073	0.734308
Na^{+}	0.2150201	1.686356
Ca^{2+}	0.2577062	2.029290

Table S2: Metal ions LRR-DE optimized parameters for the 12-6-1 model.

	C^{-6} (kJ mol^{-1} nm^{6})	C^{-12} (kJ mol^{-1} nm^{12})	q (e)
Zn^{2+}	-0.004349	3.405e-08	2.300773
Ni^{2+}	-0.000057	1.232e-07	2.213392
Mg^{2+}	-0.005197	3.344e-08	2.321638
Na^{+}	0.000620	3.689e-07	1.021000
Ca^{2+}	-0.008399	6.562e-07	2.271904

Table S3: Metal ions LRR-DE optimized parameters for the 12b-1-E1Gr model.

	C1 (kJ mol^{-1} nm^{12})	C2 (e)	θ_1 (nm)	θ_2 (nm^{-1})	θ_3 (nm^{-2})	θ_4 (nm)
Zn^{2+}	2.912e-05	696.482913	-0.099025	15.281931	0.270012	0.126974
Ni^{2+}	4.1724190	4.9229e-07	-0.021800	10.000000	7.000000	0.100000
Mg^{2+}	-22.109731	-91.616616	-0.795994	20.000000	10.00000	0.270071
Na^{+}	5.782e-06	2.4124543	-0.057371	8.4124410	6.089116	0.182687
Ca^{2+}	1.085e-04	11.3382033	-0.101856	10.1049636	8.342623	0.218861

References

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