Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

A Theoretical Study on Mixtures of Amino Acid-Based Ionic Liquids

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Table S1. Atomic charges, *q*, for the force field parameterizations of ions studied in this work

[EMIM]		[CH]		[MP]		[GLY]		[ALA]		[SER]		[PALA]	
#	*q*	#	*q*	#	*q*	#	*q*	#	*q*	#	*q*	#	*q*
1	-	1	0.1140	1	-0.0470	1	-1.0580	1	-1.0774	1	-1.0699	1	0.1120
2	-	2	-0.2800	2	0.1080	2	0.4529	2	0.5784	2	0.4821	2	-0.1280
3	0.1696	3	-0.2800	3	-0.1320	3	0.8245	3	0.7508	3	0.7739	3	-0.1090
4	-	4	-0.2800	4	-0.4430	4	-0.8250	4	-0.8155	4	-0.7967	4	-0.1660
5	0.0629	5	0.1580	5	-0.0460	5	0.3172	5	0.3123	5	0.3394	5	-0.0590
6	0.2110	6	0.1580	6	0.1080	6	-0.8671	6	-0.8343	6	-0.8230	6	-0.1130
7	0.2002	7	0.1580	7	-0.0570	7	0.3429	7	0.3379	7	0.3420	7	-1.0520
8	0.2121	8	0.1580	8	0.2840	8	-0.0897	8	-0.1178	8	-0.1166	8	0.7480
9	-	9	0.1580	9	0.2840	9	-0.0977	9	-0.0511	9	0.3655	9	0.6620
10	0.1388	10	0.1580	10	0.0980			10	-0.0455	10	-0.7238	10	-0.8070
11	0.1438	11	0.1580	11	0.0980			11	-0.0372	11	-0.0744	11	0.3350
12	0.1367	12	0.1580	12	0.0780			12	-0.0005	12	-0.0670	12	-0.7770
13	0.0782	13	0.1580	13	0.0780					13	0.3685	13	0.2890
14	0.0618	14	-0.0520	14	0.0980							14	-0.1680
15	0.0621	15	0.3030	15	0.0980							15	0.0070
16	-	16	0.1270	16	0.0780							16	-0.0990
17	0.0838	17	0.1270	17	0.0780							17	-0.0480
18	0.0480	18	0.0110	18	0.0790							18	0.0490
19	0.0478	19	0.0110	19	0.0790							19	0.1550
		20	-0.6970	20	0.0790							20	0.0450
		21	0.4740									21	0.0640
												22	0.0580

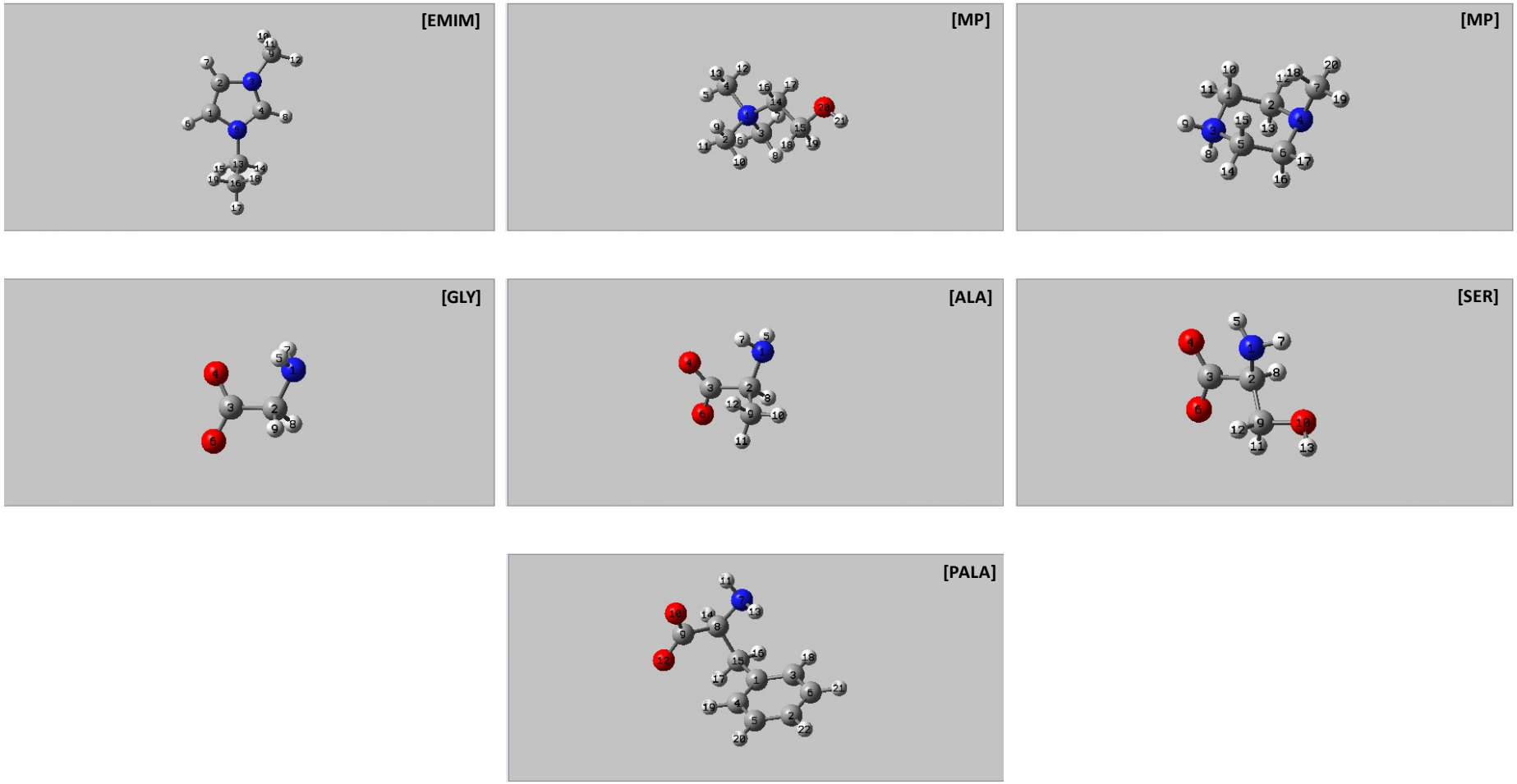

Fig. S1 Atom labeling used in Table S1 for the studied ions.

Table S2. Systems considered for NPT molecular dynamics simulations. *x* stands for anion mole ratio, *p* for pressure, *T* for temperature and *N* for number of molecules. Subscripts of anions indicate anion mole ratio, and those for cations cation mole ratio.

- **Mixtures $[EMIM][GLY]_x[ANI2]_{1-x}$ ([ANI2]=[ALA] or [SER] or [PALA])**

	N				
x	[EMIM]	[GLY]	[ANI2]	*p* / bar	*T* / K
0	400	–	400	1	300
0.1	400	40	360	1	300
0.2	400	80	320	1	300
0.3	400	120	280	1	300
0.4	400	160	240	1	300
0.5	400	200	200	1	300
0.6	400	240	160	1	300
0.7	400	280	120	1	300
0.8	400	320	80	1	300
0.9	400	360	40	1	300
1	400	400	–	1	300

- **Mixture $[EMIM][GLY]_{0.25}[ALA]_{0.25}[SER]_{0.25}[PALA]_{0.25}$**

N						
[EMIM]	[GLY]	[ALA]	[SER]	[PALA]	*p* / bar	*T* / K
400	100	100	100	100	1	300

- **Mixture $[EMIM]_{0.33}[CH]_{0.33}[MP]_{0.33}[GLY]$**

N					
[EMIM]	[CH]	[MP]	[GLY]	*p* / bar	*T* / K
134	133	133	400	1	300

- **$[EMIM]_{0.33}[CH]_{0.33}[MP]_{0.33}[GLY]_{0.25}[ALA]_{0.25}[SER]_{0.25}[PALA]_{0.25}$**

N								
[EMIM]	[CH]	[MP]	[GLY]	[ALA]	[SER]	[PALA]	*p* / bar	*T* / K
134	133	133	100	100	100	100	1	300

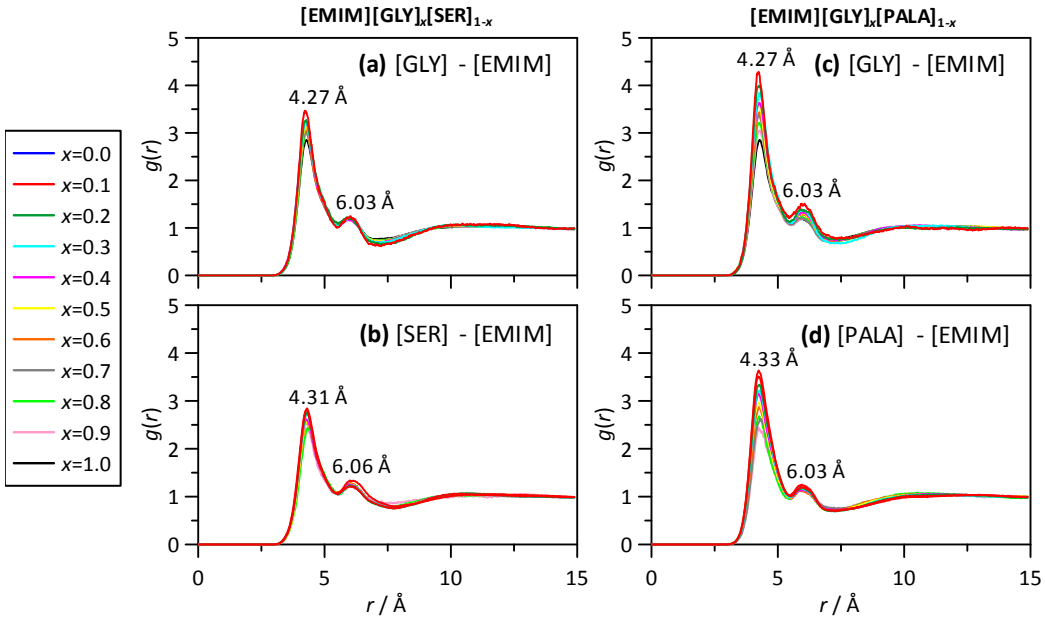

Fig. S2 Center-of-mass radial distribution functions, $g(r)$, for the reported ionic pairs in the reported mixed ionic liquids at 300 K and 1 bar.

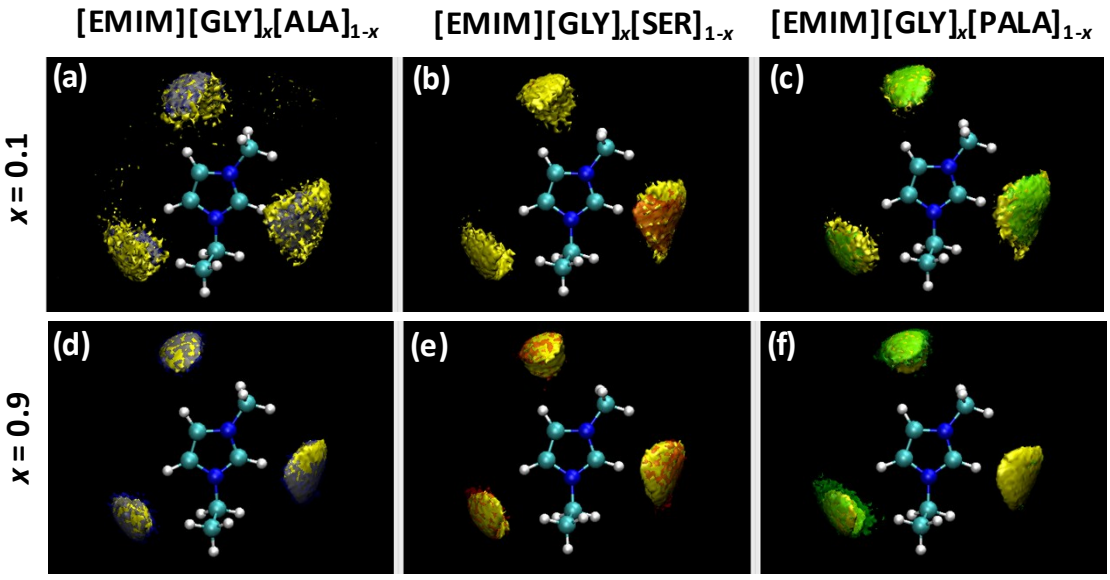

Fig. S3 Spatial distribution functions around [EMIM] cation for the carbon atoms in COO group of anions in the reported mixed ionic liquids at 300 K and 1 bar. Color code: (yellow) C in COO of [GLY], (blue) C in COO of [ALA], (red) C in COO of [SER], and (green) C in COO of [PALA].

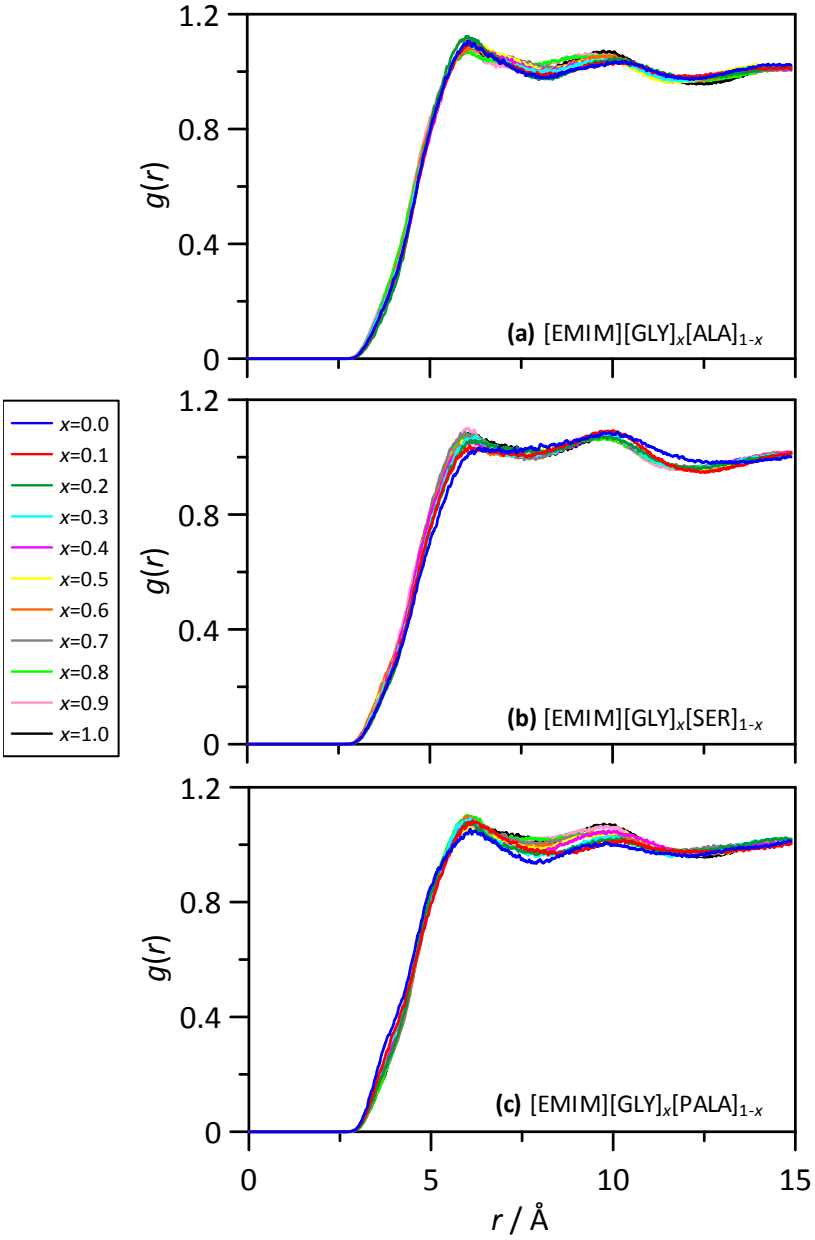

Fig. S4 Radial distribution functions, $g(r)$, between nitrogen atoms in imidazolium ring of [EMIM] cation, for the reported mixed ionic liquids at 300 K and 1 bar.