Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.

Electronic Supplementary Information for: Assessing the Reliability of Computing Ion Pair Lifetimes and Diffusivity to Predict Experimental Viscosity Trends of Ionic Liquids

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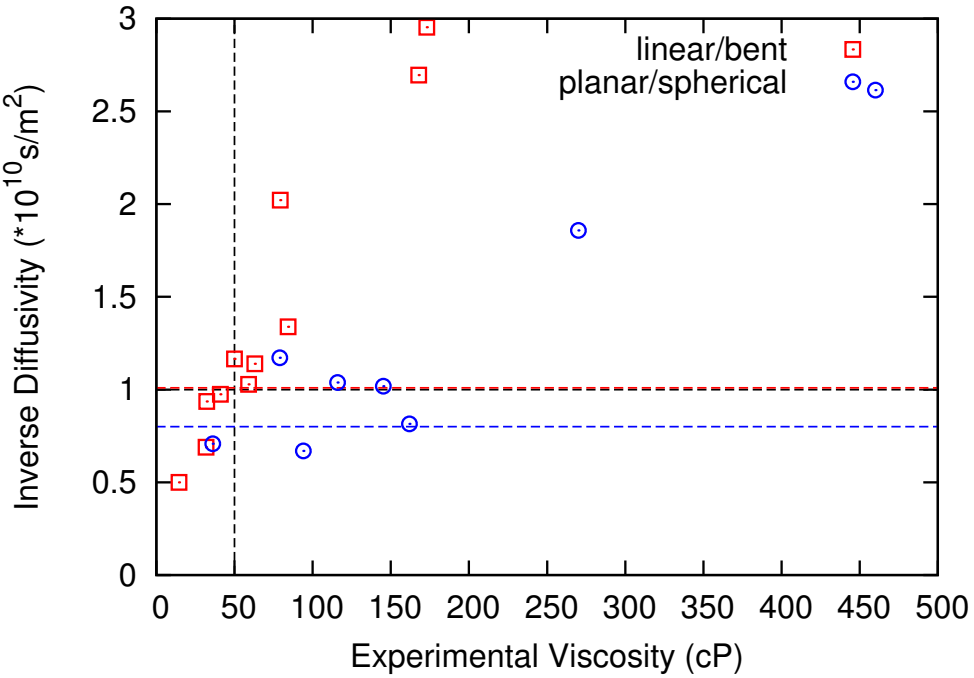

Figure S1: Inverse self-diffusivity vs experimental viscosities for selected ILs. Dashed lines represent various cutoffs used in predictions. The uncertainty estimates were smaller than the symbol size and thus excluded for clarity. Diffusivities were corrected for system size effects using viscosities obtained from a Vogel-Fulcher-Tammann fitting of experimental viscosities

Table S1: All experimental(298 K) and computed (400 K) data used in the analysis. Viscosities have units of cP, ion pair lifetimes have units of ps and diffusivities have units of $*10^{-11}$ m^2/s
. Empty Cells represent ionic liquids without Vogel-Fulcher-Tammann parameters so system size corrections were not possible

Ion Pair	Experimental Viscosity	Ion Pair Lifetime	Diffusivity (uncorrected)	Diffusivity (Corrected)	Group
[C4C1IM] [NTF2]	50 [1]	699 ± 8	4.7 ± 0.9	8.5 ± 0.9	Linear/Branched
[C2C1IM] [NTF2]	32.2 [2]	488 ± 7	6.3 ± 2.0	10.7 ± 2.0	Linear/Branched
[C4C1PYR] [NTF2]	79.3 [3]	1597 ± 72	2.0 ± 0.4	4.9 ± 0.4	Linear/Branched
[C4C1PY] [NTF2]	63 [4]	678 ± 35	5.4 ± 1.1	8.8 ± 1.1	Linear/Branched
[C4PY] [NTF2]	59.0 [5]	604 ± 6	5.9 ± 1.5	9.7 ± 4.5	Linear/Branched
[C4C1PIP] [NTF2]	173 [6]	3146 ± 335	0.9 ± 0.2	3.4 ± 0.2	Linear/Branched
[P2228] [NTF2]	129 [7]	1793 ± 197	2.3 ± 0.2		Linear/Branched
[C4C1IM] [OTF]	84.3 [1]	706 ± 29	4.3 ± 1.1	7.5 ± 1.1	Linear/Branched
[C2C1IM] [OTF]	41 [8]	433 ± 12	6.0 ± 1.4	10.3 ± 1.4	Linear/Branched
[C4C1PYR] [OTF]	167.8 [9]	1636 ± 31	1.3 ± 0.2	3.7 ± 0.2	Linear/Branched
[C4C1IM] [DCA]	31.8 [10]	365 ± 34	8.8 ± 0.9	14.5 ± 0.9	Linear/Branched
[C2C1IM] [DCA]	14.5 [11]	249 ± 29	12.3 ± 1.3	20.0 ± 1.3	Linear/Branched
[P2224] [DCA]	60 [12]	294 ± 15	11.9 ± 3.7		Linear/Branched
[P2228] [DCA]	104 [12]	708 ± 51	6.6 ± 1.8		Linear/Branched
[C4C1IM] [PF6]	261 [13]	852 ± 109	3.1 ± 0.8		Planar/Spherical
[C4C1IM] [BF4]	116 [13]	496 ± 48	6.0 ± 1.0	9.6 ± 1.0	Planar/Spherical
[C2C1IM] [BF4]	36.1 [11]	270 ± 8	9.2 ± 2.1	14.1 ± 2.1	Planar/Spherical
[C4C1PY] [BF4]	166.7 [14]	455 ± 13	6.7 ± 0.9		Planar/Spherical
[C4PY] [BF4]	145.2 [14]	458 ± 112	6.8 ± 1.3	9.8 ± 1.3	Planar/Spherical
[C4C1IM] [CNPYR]	162 [15]	514 ± 165	8.1 ± 0.8	12.2 ± 0.8	Planar/Spherical
[C2C1IM] [CNPYR]	94 [15]	283 ± 52	11.2 ± 1.3	14.9 ± 1.3	Planar/Spherical
[C4C1IM] [4TRIZ]	270 [15]	980 ± 47	2.7 ± 0.3	5.4 ± 0.3	Planar/Spherical
[C2C1IM] [4TRIZ]	79 [15]	447 ± 5	5.2 ± 0.5	8.5 ± 0.5	Planar/Spherical
[C4C1PYR] [4TRIZ]	460 [15]	2099 ± 163	1.1 ± 0.1	3.8 ± 0.1	Planar/Spherical

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