Supporting Materials for
Dynamics in an Idealized Ionic Liquid Model

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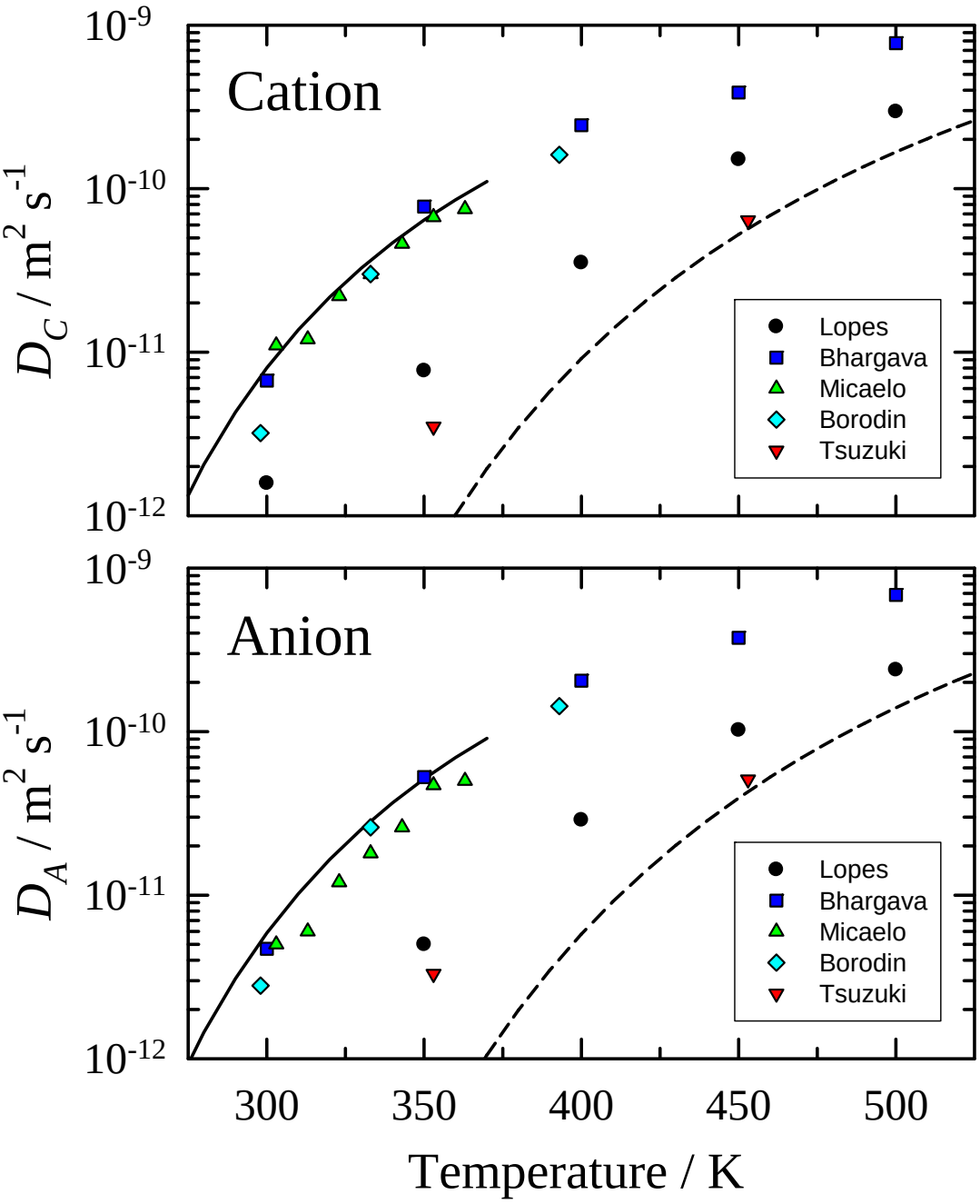

Fig. S1: Comparison of simulated and experimental diffusion coefficients of $[Im_{41}][PF_6]$. The solid and dashed curves are the experimental parameterization of *D* by Tokuda *et al.*[1] and the fitted *D*(*T*) curve of the model from Fig. 3. The points are from simulations using the all-atom representations of $[Im_{41}][PF_6]$ developed by Lopes *et al.*[2,3] Bhargava *et al.*[3], Micaelo *et al.*,[4] Borodin,[5] and Tsuzuki *et al.*[6] Note that only simulations that have been run for sufficient times (at least several ns) to be expected to provide accurate diffusion coefficients have been included in this figure.

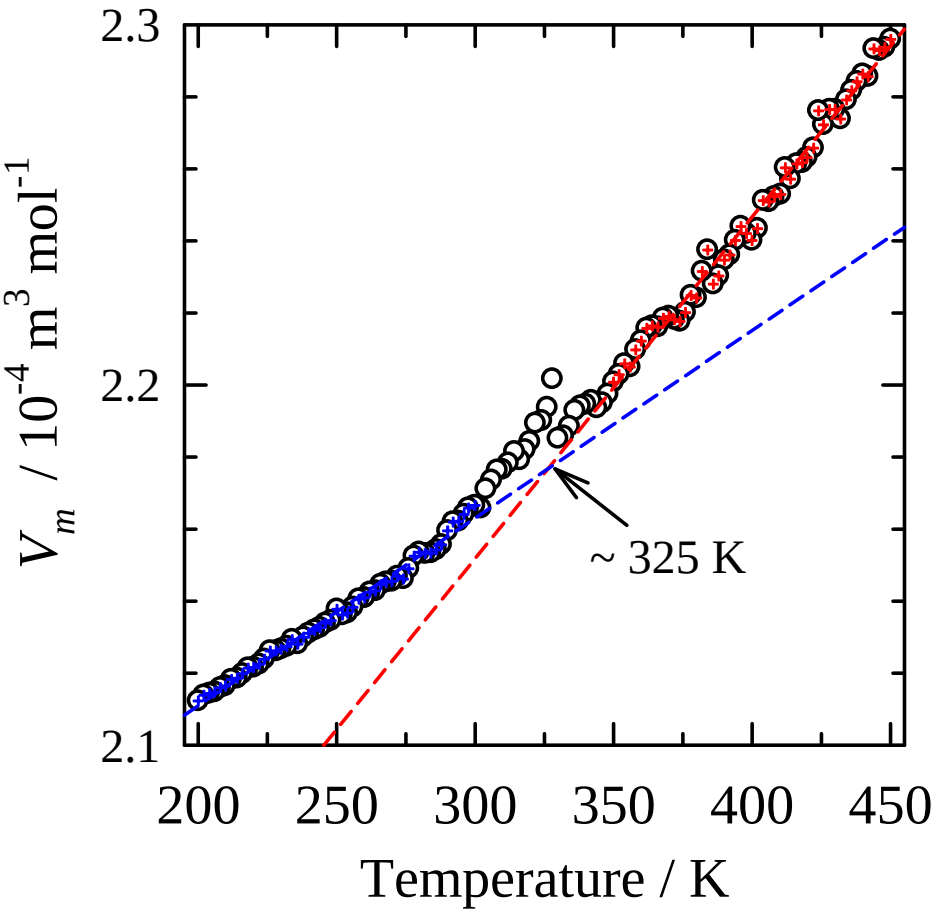

Fig. S2: Volume dependence observe in a simulated cooling run from an equilibrated 450 K sample cooled at a rate of 2 K/ns. As shown by the red and blue points, the data can be characterized by high- and low-temperature regions in which the molar volume is linear in temperature. The extrapolations of these regions intersect at 325 K suggesting a model T_g somewhat below this temperature. We note that T_g of $[Im_{41}][PF_6]$ is ~191 K[7] and therefore this crude estimate of the model T_g is consistent with the ~100 K displacement between corresponding states of the model and experimental systems inferred from Fig. 5.

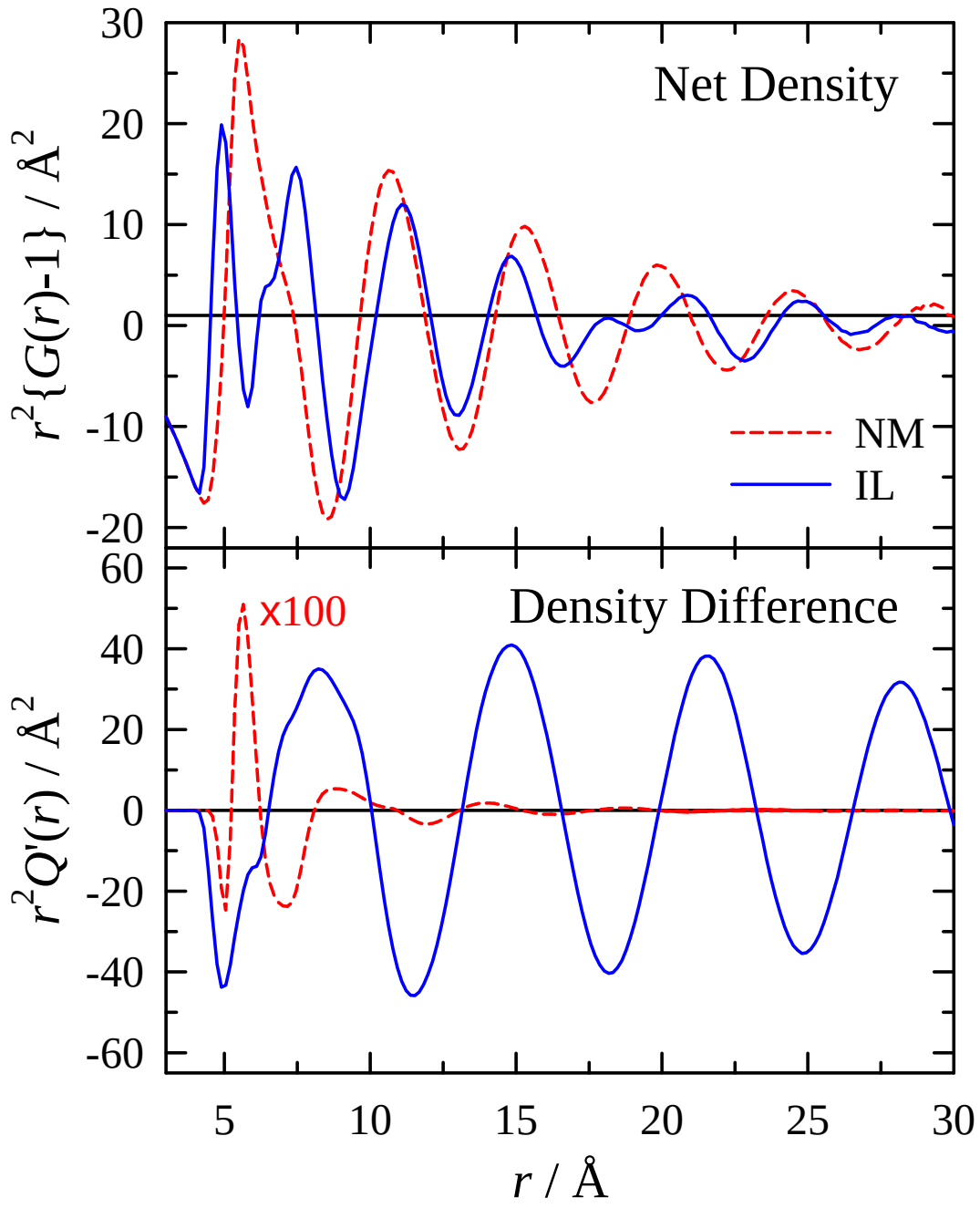

Fig. S3: Comparison of the total density distribution $G(r) = \frac{1}{4}\{g_{CC}(r) + g_{AA}(r) + 2g_{CA}(r)\}$ and the density difference distribution $Q'(r) = \frac{1}{4}\{g_{CC}(r) + g_{AA}(r) - 2g_{CA}(r)\}$ in the IL and NM systems at 450 K. Note that $Q'(r)$ is simply proportional to $Q(r)$, the charge density distribution defined in Section 3 (Fig. 4) for the IL. These functions have been multiplied by r^2 to emphasize their long-time behavior. $Q'(r)$ for the NM has been multiplied by a factor of 100 to make it visible here.

Table S1: Coordination Numbers in the IL and NM Systems at 450 K

R/Å	N_{CC}	N_{AA}	N_{CA}	*G*	*Q'*
Ionic Liquid					
8.0	4.9	5.1	6.2	5.6	-0.6
13.2	23.1	22.1	26.6	24.6	-2.0
18.7	71	70	73	72	-1.0
Neutral Mixture					
R/Å	C-C	A-A	C-A	G	Q
8.0	5.1	5.4	5.6	5.4	-0.2
13.2	24.5	24.5	24.6	24.6	-0.1
18.7	71	71	71	71	0.0

The columns labeled N_{ij} are coordination numbers obtained by integrating the center of mass distributions shown in Fig. 14 to the radii *R* listed:

$$N_{ij}(R) = 4\pi\rho\int_0^R r^2 g_{ij}(r)dr \qquad \text{(S1)}$$

G and *Q*' refer to the composite density distributions defined in Fig. S3.

References:

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