Comparative Molecular Dynamics Simulation Studies of Simple and Polymerized Ionic Liquids: Electronic Supplementary Information (ESI)

Arshid Ahmad,[1] Robin Köster,[1] Sebastian Kloth,[1] and Michael Vogel[1, a)]

Institute for Condensed Matter Physics, Technische Universität Darmstadt, Hochschulstr. 6, 64289 Darmstadt, Germany

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[a)]Electronic mail: michael.vogel@pkm.tu-darmstadt.de

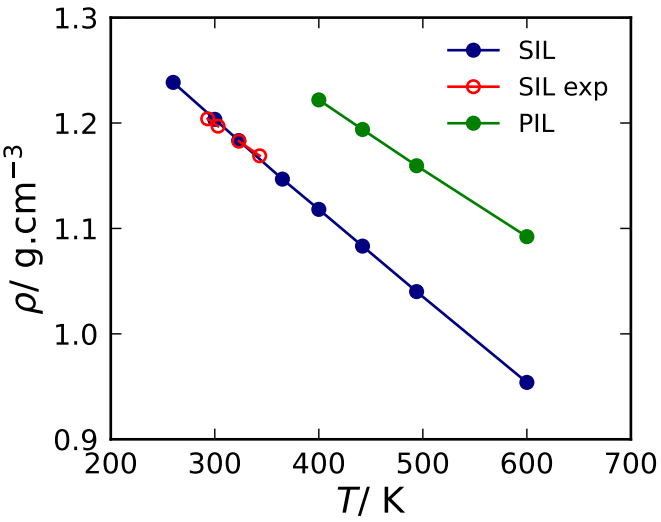

Figure S1. Temperature-dependent density of the simulated simple ionic liquid (SIL) and polymerized ionic liquid (PIL). For comparison, experimental data (red) for the SIL are included.

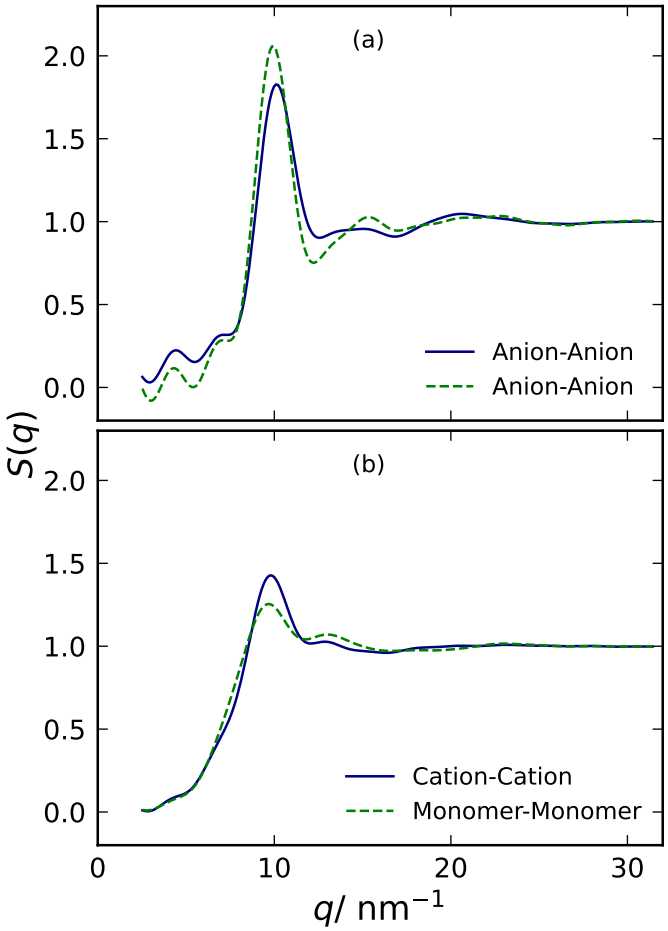

Figure S2. Partial static structure factors $S_{\mathrm{AB}}(q)$ of the simulated SIL (navy) and PIL (green) at 400 K: (a) anion-anion and (b) cation-cation (SIL) or monomer-monomer (PIL). The partial structure factors were obtained by Fourier transformation from the corresponding radial distribution functions $g_{\mathrm{AB}}(r)$, which were calculated using the respective center-of-mass positions in the main text.

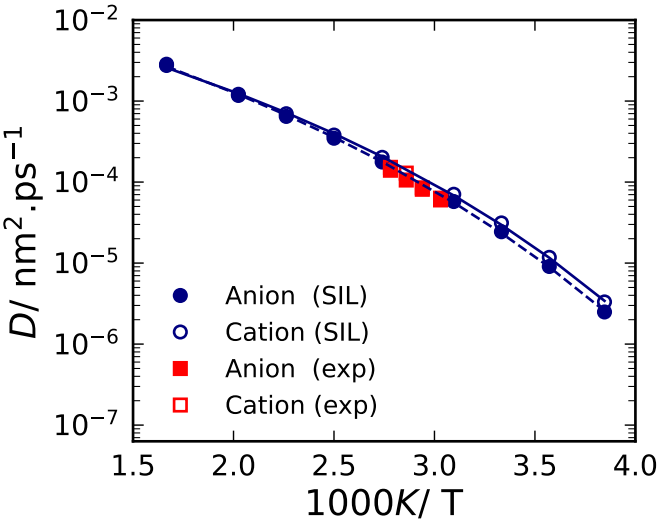

Figure S3. Self-diffusion coefficients D of cations (solid symbols) and anions (open symbols) in the simulated SIL, see main text, and corresponding data from experimental studies (red).[1] The experimental data (unpublished) were obtained from ^{1}H and ^{19}F NMR field-gradient studies. Information about the methodology and setup of these measurements can be found in previous NMR work on other ionic liquids.[2]

REFERENCES

[1]E. Steinrücken and M. Vogel, (unpublished data).

[2]M. Becher, E. Steinrücken, and M. Vogel, J. Chem. Phys. **151**, 194503 (2019).