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Ionic Liquids with Fluorinated Block-Oligomer Tails: Influence of Self-Assembly on Transport Properties

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Supplementary Information

The chemical structure and ^{1}H NMR spectrum of ZMeImI are shown in Fig. S1a and Fig. S1b, respectively.

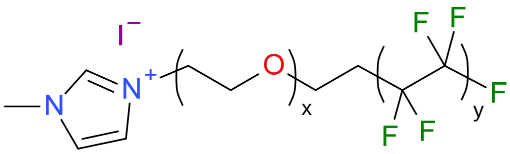

Fig. S1a Chemical structure of ZMeImI. The average values of *x* and *y* are about 6.5±0.5 and 3.5±0.5, respectively.

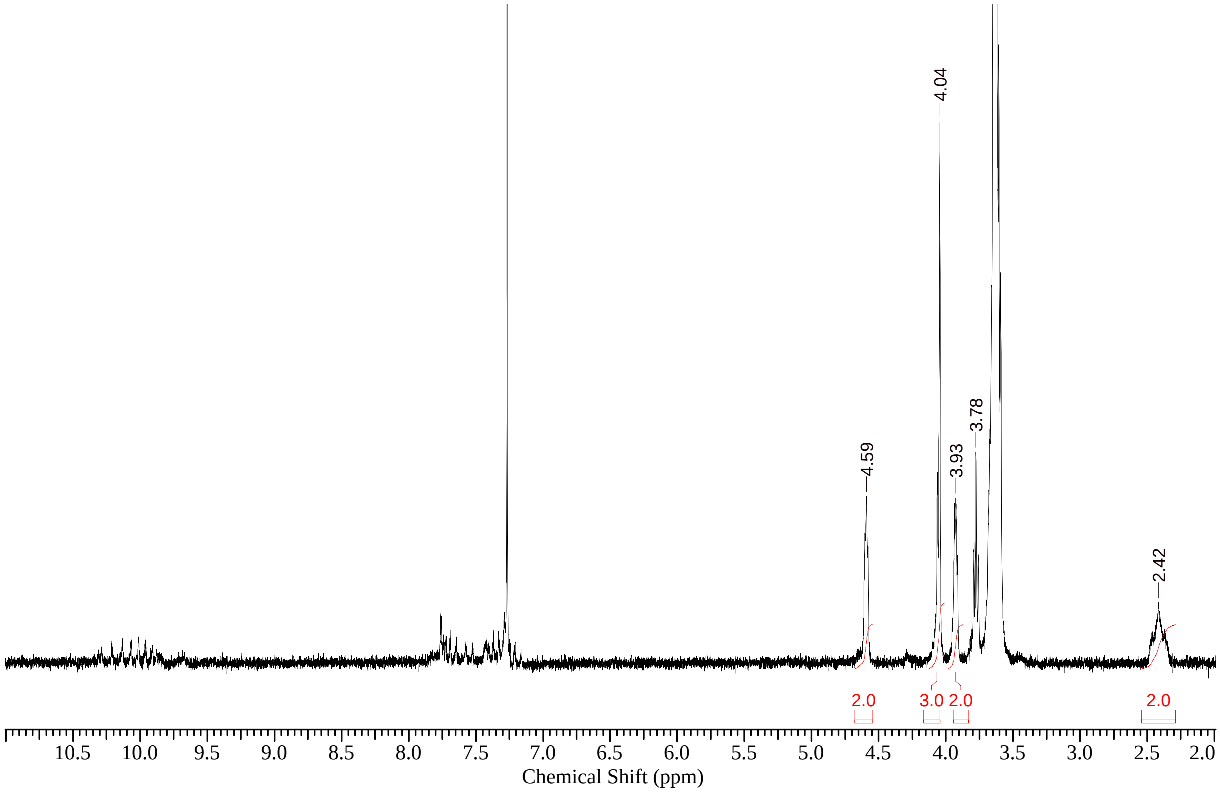

Fig. S1b ^{1}H NMR spectrum of ZMeImI. δ_H (400 MHz; $CDCl_3$; Me_4Si) 10.43–9.76 (m, N^+CHN), 7.89–7.10 (m, NCH and N^+CH), 4.59 (t, J = 4 Hz, 2H, N^+CH_2), 4.04 (s, 3H, NCH_3), 3.93 (t, J = 4.4 Hz, 2H, $N^+CH_2\mathit{CH_2}O$), 3.84–3.50 (br s, 23H, $CH_2\mathit{CH_2}O$), 2.49–2.32 (br m, 2H, CH_2CF_2).

Figs. S2 to S8 show the shear stress vs. shear rate plots, at selected temperatures, for ZMeImI, ZMeImTf$_2$N, mPEG16MeImI, mPEG12MeImI, mPEG7MeImI, Zonyl® FSO-100 (ZOH), and monomethoxy-terminated PEG with an average molecular weight of 550 g/mol (mPEG12OH). ZMeImTf$_2$N, the mPEG*n*MeImI ILs, ZOH, and mPEG12OH showed a Newtonian behavior, that is, a linear variation of shear stress with shear rate, over a temperature range of 25 to 95 °C. The viscosity of ZMeImI could be determined only at temperatures ≥ 85 °C, and the shear stress vs. shear rate relationship was non-linear (*cf.* Fig. S2).

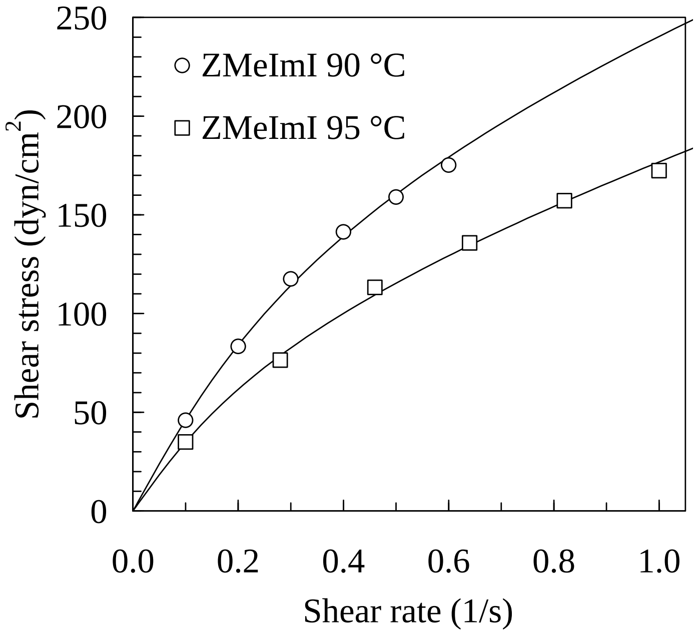

Fig. S2 Shear stress vs. shear rate plots for ZMeImI at 90 and 95 °C. The lines represent the Powell–Eyring fits. According to the Powell–Eyring model, $(\eta - \eta_\infty)/(\eta_0 - \eta_\infty) = \sinh^{-1}(\theta\dot{\gamma})/(\theta\dot{\gamma})$, where η is the viscosity at shear rate, $\dot{\gamma}$, η_0 is the zero-shear-rate viscosity, η_∞ is the viscosity as $\dot{\gamma} \to \infty$, and θ is a temperature-dependent relaxation time.

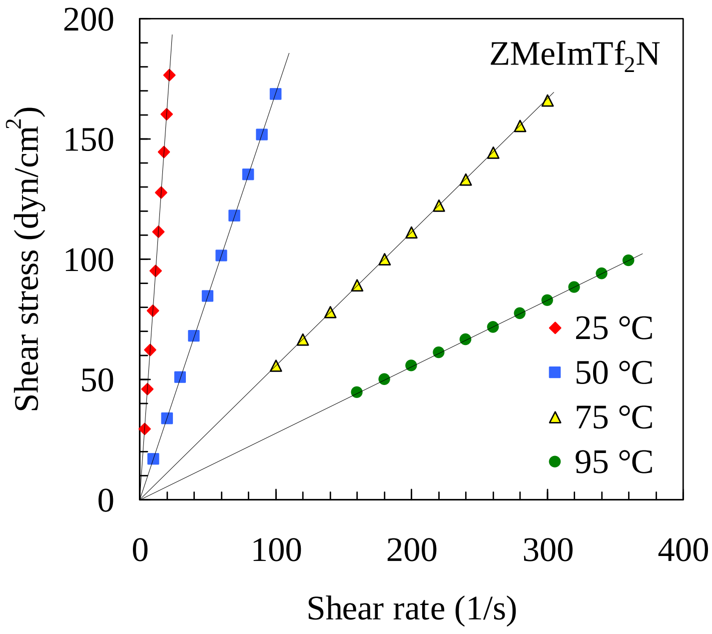

Fig. S3 Shear stress vs. shear rate plots for ZMeImTf$_2$N at 35, 50, 75, and 95 °C.

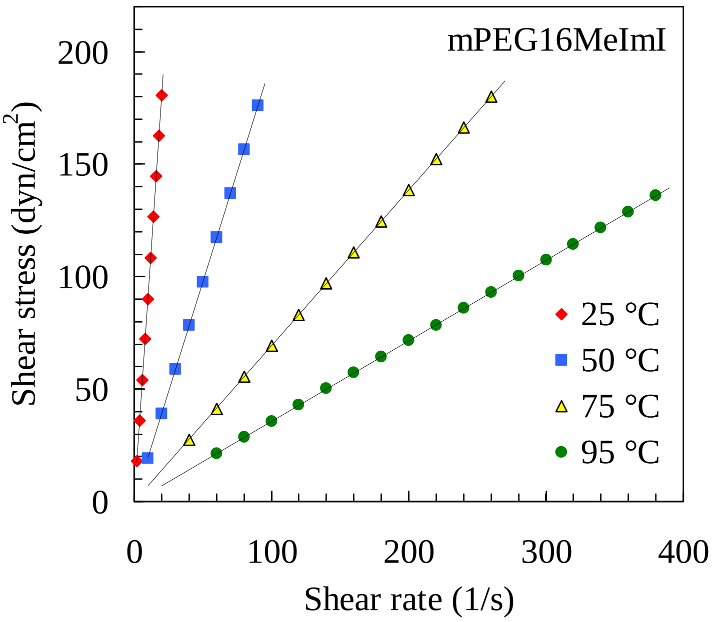

Fig. S4 Shear stress vs. shear rate plots for mPEG16MeImI at 25, 50, 75, and 95 °C.

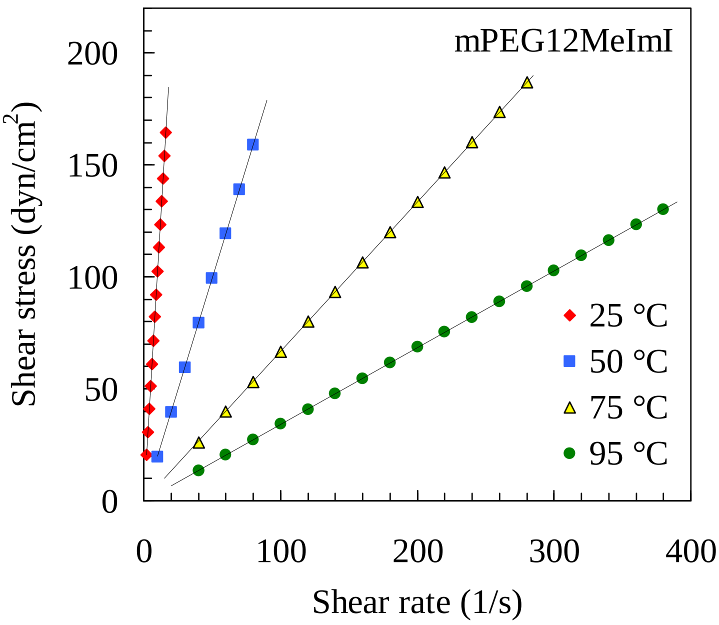

Fig. S5 Shear stress vs. shear rate plots for mPEG12MeImI at 25, 50, 75, and 95 °C.

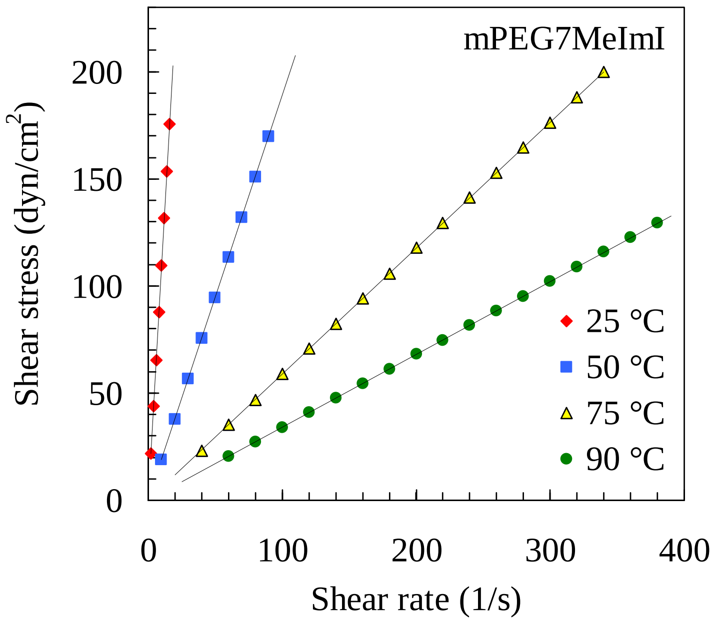

Fig. S6 Shear stress vs. shear rate plots for mPEG7MeImI at 25, 50, 75, and 90 °C.

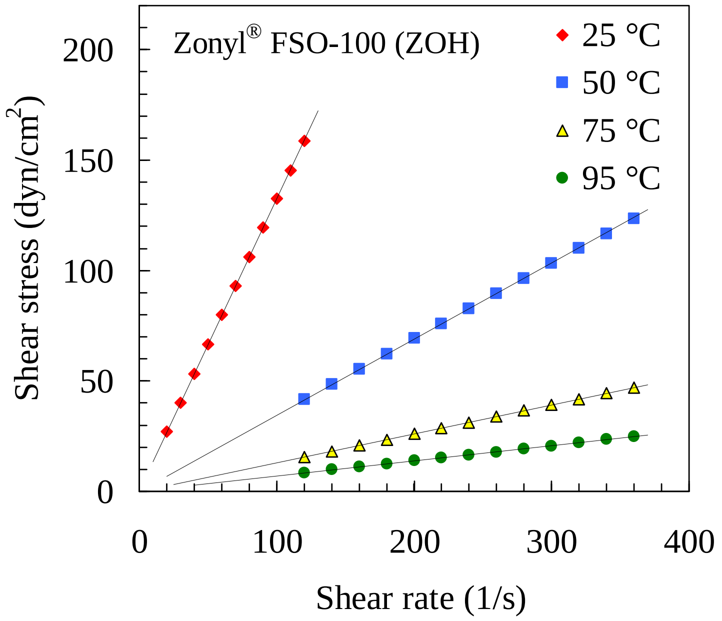

Fig. S7 Shear stress vs. shear rate plots for ZOH (Zonyl® FSO-100, CAS no. 65545-80-4) at 25, 50, 75, and 95 °C.

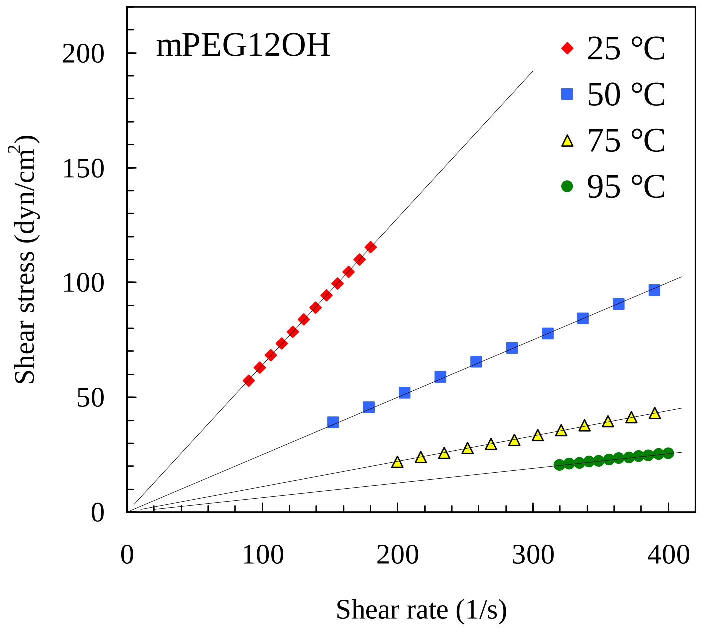

Fig. S8 Shear stress vs. shear rate plots for monomethoxy-terminated poly(ethylene glycol) (mPEGOH) with an average molecular weight of 550 g/mol ($CH_3(OCH_2CH_2)_{12}OH$, CAS no. 9004-74-4, Aldrich) at 25, 50, 75, and 95 °C.

Fig. S9 shows a schematic of the electrolyte film used in the self-consistent mean field lattice simulations. The lattice is shown by the hatched square with sides denoted by *a*, *b*, *c*, and *d*. The corner of the square lattice, denoted by *O*, corresponds to *X* = 0 and *Y* = 0. *O* is located at the mid-section along the thickness of the film. Side *a* represents the electrolyte–vacuum interface. The letter V indicates vacuum or void. Periodic boundary conditions were used on sides *b* and *d*, and a reflecting boundary condition was used on side *c* of the square. It was assumed that there were no composition gradients along the *Z* axis of the coordinate system. The results of our simulations showed that the planes of the lamellae, or the axes of the cylinders, were oriented parallel to the electrolyte–vacuum interface. The cylinder axes were parallel to the *Z* axis.

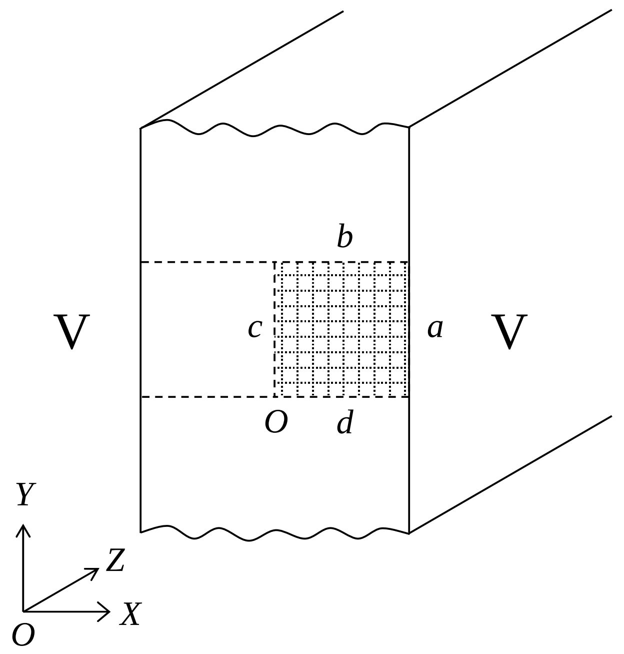

Fig. S9 A schematic of the electrolyte film modeled in the SCMF simulations.