

Evolution of Ionic Liquid Nanostructures in Mixtures: Implications for Thermophysical Properties

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Abstract. Ionic liquids (ILs) exhibit complex nanoscale organization arising from competing electrostatic and van der Waals interactions, resulting in intermediate-range structural ordering that can strongly influence their thermophysical properties. Understanding how this organization evolves upon the addition of molecular solutes, and how these structural changes affect macroscopic transport properties, remains an important challenge in the study of complex liquids. In this work, we investigate the relationship between nanoscale structure and thermal conductivity in mixtures of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C₂C₁im][TFSI]) with two hydrofluorocarbons (HFCs): difluoromethane (HFC-32) and 1,1,1,2-tetrafluoroethane (HFC-134a).

High-pressure small- and wide-angle X-ray scattering (SAXS/WAXS), coupled with molecular dynamics (MD) simulations, is used to characterize the composition-dependent evolution of ionic ordering. Scattering measurements reveal a characteristic charge-ordering peak near 0.9 Å⁻¹, which persists at low and moderate HFC concentrations despite substantial dilution of the IL. At higher HFC concentrations, this peak broadens and diminishes, indicating progressive disruption of intermediate-range ionic correlations. Complementary spectroscopy measurements, radial distribution functions, coordination numbers, and ion-clustering analyses demonstrate that local ionic associations persist even after the extended ionic network loses connectivity.

These structural changes are correlated with experimental thermal conductivity measurements and molecular-level heat flux decomposition from nonequilibrium MD simulations. At low and moderate HFC concentrations, the persistence of the extended ionic network supports interaction-dominated heat conduction, resulting in a weak composition dependence of thermal conductivity. Beyond approximately 80 mol% HFC, fragmentation of the ionic network coincides with a pronounced reduction in the bonded contribution to heat conduction and an increasing contribution from molecular transport. The results demonstrate that extended ionic-network connectivity, rather than local ion association alone, is a critical structural descriptor governing thermal transport in these mixtures. More broadly, this work highlights the importance of combining scattering techniques with molecular simulations to establish structure–property relationships in complex ionic fluids.

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10:45 AM (UTC-05:00) Eastern Time (US & Canada) | Hybrid format, remote presentation

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