What room temperature ionic liquids teach us about the structure of liquids

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We teach our students that liquids take the shapes of their containers because molecules move freely past one another. Room temperature ionic liquids (RTILs) are salts composed of large, polarizable ions, mismatched in size and shape, so they remain liquid near room temperatures. They are under intense study as potential electrolytes in lithium-ion batteries. Small-angle X-ray scattering (SAXS) experiments show "polar scattering domains" in RTILs, but interpretation of experimental data is challenging. Our group recently developed a model using SAXS line shapes to establish unambiguously that "polar scattering domains" in RTILs are polar aggregates of cations and anions, derive distances between ions within polar aggregates, and estimate for the first time from experimental data the size of polar aggregates in RTILs. Further work shows that the polar aggregates in RTILs adopt local structures similar to those of the analogous crystalline solid. Thus, RTILs require us to revise our simple picture of liquid structure. Possible extensions of our model to gain insights into thermodynamics and transport properties of liquids will also be described.

Bio

Ralph Wheeler earned a BS degree in chemistry from Harvey Mudd College, a PhD in computational chemistry from Cornell University, and completed 2 years of postdoctoral training with Andy McCammon at the University of Houston. He served on the faculty of the University of Oklahoma for 20 years before becoming Chair of the Chemistry and Biochemistry Department at Duquesne University in Pittsburgh for six years. He currently serves as a professor of chemistry at Northern Illinois University, where he was Chair of the Chemistry and Biochemistry Department from 2016-2023. Along the way, he was named a Presidential Professor at the University of Oklahoma and a Fellow of the American Chemical Society. His current research spans computational materials chemistry and polymer chemistry, using quantum chemical, molecular dynamics, and QM/MM methods. His current projects include adapting signal processing methods to analyze molecular dynamics simulations and implementing quantum Monte Carlo methods to model radical reactions. Ralph has mentored 20 PhD/MS students and 31 undergraduate researchers.