Confined Water in Room-Temperature Ionic Liquids by Small-Angle Neutron Scattering

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Room-temperature ionic liquids (RTILs) are fascinating solvents to design as we desire. In addition, additives into the RTILs can enlarge the usage of the functional solutions. Here, we focus on the RTILs-water mixtures, which can control protein folding and its hyperstructure [1, 2].

Very recently, direct evidence of confined water (water pocket) inside RTILs is obtained by complementary use of small-angle X-ray scattering and small-angle neutron scattering (SANS) [3]. The RTIL is 1-butyl-3-methylimidazolium nitrate, [C₄mim][NO₃]. Using different scattering cross section of deuteron for X-ray and neutron, D₂O is enhanced in the [C₄mim][NO₃]-D₂O mixtures. The distinct peak in SANS corresponds to the 3 nm-sized water pocket even at the water-rich region. The simulated water pocket referring to the observed SANS profile is quite similar to water aggregations demonstrated by the molecular dynamics [4]. In the simulation box, the aggregations exist near the boundaries between polar and nonpolar nano-domains of [C₄mim][NO₃]. The theoretically predicted and experimentally obtained water pocket can explain the refolding of proteins in [C₄mim][NO₃]-D₂O [1, 2].