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

H. Abe[1#], T. Takekiyo[2], M. Shigemi[2], Y. Yoshimura[2], S. Tsuge[3], T. Hanasaki[3], K. Ohishi[4], S. Takata[5], and J. Suzuki[4]

[1]*Department of Materials Science and Engineering, National Defense Academy, Yokosuka 239-8686, Japan*

[2]*Department of Applied Chemistry, National Defense Academy, Yokosuka 239-8686, Japan*

[3]*Department of Applied Chemistry, Ritsumeikan University, Kusatsu, Shiga 525-8577, Japan*

[4]*Research Center for Neutron Science and Technology, Comprehensive Research Organization for Science and Society (CROSS), Tokai, Ibaraki 319-1106, Japan*

[5]*Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan*

 # a corresponding author: E-mail ab@nda.ac.jp

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, $[C_4mim][NO_3]$. Using different scattering cross section of deuteron for X-ray and neutron, D_2O is enhanced in the $[C_4mim][NO_3]$-D_2O 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 $[C_8mim][NO_3]$. The theoretically predicted and experimentally obtained water pocket can explain the refolding of proteins in $[C_4mim][NO_3]$-D_2O [1, 2].

[1] T. Takekiyo, K. Yamazaki, E. Yamaguchi, H. Abe, and Y. Yoshimura, J. Phys. Chem. B **116**, 11092 (2012).

[2] T. Takekiyo, Y. Koyama, K. Yamazaki, H. Abe, and Y. Yoshimura, J. Phys. Chem. B **117**, 10142 (2013).

[3] H. Abe, T. Takekiyo, M. Shigemi, Y. Yoshimura, S. Tsuge, T. Hanasaki, K. Ohishi, S. Takata, and J. Suzuki, J. Phys. Chem. Lett. **5**, 1175 (2014).

[4] W. Jiang, Y. Wang, and G. A. Voth, J. Phys. Chem. B 111, **4812** (2007).