The Experimental Evidence of the Liquid-Liquid Phase Transition in Confined Water

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Water confined in nanometer-scale pores plays a key role in various fields, such as chromatography, membrane proteins, catalysts, fuel cells, and nano technology. Thus, the structure and dynamic properties of confined water at the molecular level is essential for understanding the unique properties and the underlying mechanisms of various processes in the confined systems. Furthermore, water confined in pores of ~21 Å is not frozen in the temperature down to 140 K due to both confinement and interfacial interaction effects. This unique property of low-temperature of confined water has drawn much attention in connection with the hypothesis of the 2nd critical point between the liquid-liquid transition of bulk water proposed by simulation works. The present talk is focused on the liquid-liquid transition of water confined in mesoporous silica MCM-41 C10 whose pore diameter is 21 Å, which has been evidenced from the thermal behavior, structure and dynamic properties of confined water obtained by heat capacity, X-ray and neutron diffraction, and neutron spin echo measurements. The dynamical crossover from non-Arrhenius to Arrhenius type behavior of confined water at 220-230 K corresponds to the high-density water – the low-density water phase transition. The origin of the liquid-liquid phase transition of confined water will be discussed at the molecular level.

References

- [1] T. Yamaguchi, K. Yoshida, K. Ito, S. Kittaka, and S. Takahara, BUNSEKI KAGAKU, **60**, 115 (2011).
- [2] S. Kittaka, Y. Ueda, F. Fujisaki, T. Iiyama, and T. Yamaguchi, Phys. Chem. Chem. Phys. **13**, 17222 (2011).
- [3] K. Yoshida, T. Yamaguchi, S. Kittaka, M.-C. Bullissent-Funel, and P. Fouquet, J. Phys.: Condens. Matter **24**, 064101 (2012).
- [4] S. Kittaka, S. Takahara, H. Matsumoto, Y. Wada, T. J. Satoh, and T. Yamaguchi, J. Chem. Phys. **138**, 204714 (2013).