Soft X-Ray Absorption Spectroscopy for Observing Chemical Processes in Solution

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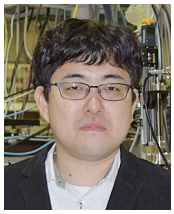

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Soft X-ray absorption spectroscopy (XAS) observes local structures of liquids with different light elements. We have developed liquid cells and devices with precise absorbance control and observed several chemical processes in solution by using *operando* XAS.[1,2] In this year, we investigated cononsolvency mechanism of polymer solutions[3] and isolated water molecules in aqueous acetonitrile solutions.[4]

1. Mechanism of Polymer Cononsolvency Explored via Oxygen K-Edge XAS

The cononsolvency of poly(*N*-isopropylacrylamide) (PNIPAM), dissolving in pure methanol and water but being insoluble in aqueous methanol solutions, was investigate by O K-edge XAS.[3] The cononsolvency emerges from the aggregation of PNIPAM with methanol clusters, leading to the collapse of the hydrophobic hydration of PNIPAM.

2. Probing Isolated Water Molecules in Aqueous Acetonitrile Solutions

O K-edge XAS of aqueous acetonitrile solutions exhibited a sharp peak around 537 eV, which was like that of water vapor and was not observed in liquid water. The inner-shell calculations revealed that the sharp peak profiles were derived not from water clusters but from isolated water molecules surrounded by acetonitrile molecules.[4] It means that the isolated water molecules in aqueous acetonitrile solutions can be analyzed using O K-edge XAS, which separates the contributions of small water clusters.

References

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2) M. Nagasaka, H. Yuzawa and N. Kosugi, *Anal. Sci.* **36**, 95–105 (2020).
3) M. Nagasaka, F. Kumaki, Y. Yao, J. Adachi and K. Mochizuki, *Phys. Chem. Chem. Phys.* **26**, 13634–13638 (2024).
4) M. Nagasaka, *J. Phys. Chem. Lett.* **15**, 5165–5170 (2024).