

Element Specific Observation of Hydration Structures in Aqueous Salt Solutions by Soft X-ray Absorption Spectroscopy

Masanari Nagasaka

Institute for Molecular Science, National Institutes of Natural Science

Summary

Microscopic properties of aqueous salt solutions such as viscosity, boiling point, and melting point, are influenced by the interaction between solute ions and solvent water molecules. Soft X-ray absorption spectroscopy (XAS) is an element specific method for light elements, where the electronic structures of ions are separately observed from those of solvent water molecules in aqueous salt solutions. Recently, we have realized XAS of liquid samples in transmission mode by developing the precise thickness control method (20 ~ 2000 nm). However, it is impossible to measure XAS of liquid samples in the low energy region below 200 eV including Li K-edge (60 eV) and Cl L-edge (200 eV) since transmitted soft X-rays mostly consist of high order X-rays due to the small transmission of first order X-rays. The experiments were performed at soft X-ray beamline BL3U at the UVSOR-III Synchrotron. From O K-edge XAS of aqueous LiCl solutions, the peak related to water molecules in the first coordination shells of Li⁺ ions shows a lower energy shift by increasing the salt concentration until 8 M, but it shows a higher energy shift above 8 M. This behavior would be caused by the interaction of Cl⁻ ion to the hydration shell of Li⁺ ion at the high concentration region. On the other hand, we have established soft X-ray transmission argon gas window that removes higher order X-rays above 240 eV and have developed an ultrathin liquid cell for obtaining the high photon flux of first order X-rays below 200 eV. By using these techniques, we have obtained XAS spectra of 2 M LiCl solutions at the Li K-edge and Cl L-edge though a signal-to-noise ratio is still not enough. In the future, we will measure XAS of aqueous LiCl solutions with a high precision by increasing the photon flux of first order X-rays. The hydration shell of Li⁺ ions will be investigated from both Li⁺ ions and hydrating water molecules by XAS at the Li and O K-edges.