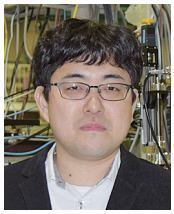
Soft X-Ray Absorption Spectroscopy for Observing Chemical Processes in Solution

Department of Photo-Molecular Science
Division of Photo-Molecular Science III



NAGASAKA, Masanari
Assistant Professor

Chemical processes in solutions were investigated using *operando* soft X-ray absorption spectroscopy (XAS) with different light elements.[1,2] In this year, the metal-ligand delocalization of metal porphyrin complexes was investigated from the ligand side,[3] and inner-shell calculations of large molecular systems were developed for polymers in solutions.[4]

1. Metal-Ligand Delocalization of Metal Porphyrin Complexes in Solutions

Metal-ligand delocalization of metal porphyrin complexes such as iron protoporphyrin IX was proved from the ligand side using N K-edge XAS.[3] The C=N π* peaks of porphyrins are useful for discussing the central metal dependence of metal-ligand delocalization and the hydration structures of metal porphyrins in solutions.

2. Inner-Shell Calculations of Polymers in Solutions

Inner-shell spectra of poly(*N*-isopropylacrylamide) (PNIPAM) in solutions were calculated by extracting the 5-mer PNIPAM chains with terminated H atoms, including the second coordination shells of solvent molecules, from the snapshots of the molecular dynamics simulations.[4] The C=O π* peaks of PNIPAM at the O K-edge reflected the structural changes of the polymer chains and the coordination of the C=O groups with solvent methanol and water molecules.

References

1) M. Nagasaka and N. Kosugi, *Chem. Lett.* **50**, 956–964 (2021).
2) M. Nagasaka, H. Yuzawa and N. Kosugi, *Anal. Sci.* **36**, 95–105 (2020).
3) M. Nagasaka, S. Tsuru and Y. Yamada, *Phys. Chem. Chem. Phys.* **26**, 23636–23645 (2024).
4) M. Nagasaka, Y. Yao and K. Mochizuki, *J. Chem. Phys*. **162**, 054901 (8 pages) (2025).