Structure Estimation from XANES spectra using machine learning

([1]*Graduate School of Science, Tohoku University*, [2]*Innovation Research Center for Fuel Cells, The University of Electro-Communications,* [3]*Institute of Materials Structure Science High Energy Accelerator Research Organization (KEK)*, [4]*School of High Energy Accelerator Science, SOKENDAI,* [5]*Graduate School of Science and Engineering, Ibaraki University*)
○Kentaro Fuku,[1] Takefumi Yoshida,[2] Hitoshi Abe,[3,4,5] Hiroaki Iguchi,[1] Shinya Takaishi[1]
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In coordination chemistry, the only methods for structure estimation have been single crystal X-ray structure analysis or DFT calculations. Recently, X-ray absorption fine structure (XAFS) has been attracting attention as a method for estimating coordination environments. However, the use of XAFS (especially XANES) in coordination chemistry is not common technique, and the most of its use are limited to "fingerprint matching" such as comparison with reference samples. In this study, we measured the XAFS spectra of Ni complexes, and aimed to estimate the coordination environment conveniently by spectral clustering using machine learning. As a result of our experiments, we succeeded in cluster partitioning by the number of coordination and the chemical environment of the coordinating atoms. And the clusters to which they belonged were changed following the ligand exchange reaction by adding ligands. These results suggest that the combination of XANES and machine learning will make it possible to estimate the coordination environment more easily.