

Miao Wang<sup>1</sup>, Ken Sakaushi<sup>1</sup>

<sup>1</sup>National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

# キーワード : Electrocatalysis, Noble metal, Local structure, Atomic coordination

# 1. 背景と研究目的

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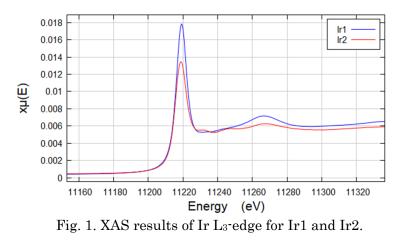
Highly efficient electrocatalytic materials are of great importance for green chemical industry to produce high-value chemicals<sup>[1]</sup>. To achieve a rational design of electrocatalysts, the clarification of their local structures, especially from an electronic/atomic point of view for low-loading catalytic species, is critical but still challenging. In this research, we used synchrotron-based X-ray absorption spectroscopy (XAS) to reveal the local structures of two typical low-loading Ir-based electrocatalysts. The disclosed electronic and atomic configurations for Ir will benefit the comprehensive understanding of the structure-performance relationship for synthesizing superior electrocatalysts.

### 2. 実験内容

Ir-based electrocatalysts were prepared as films. Fluorescence detection mode was adopted to collect the Ir  $L_3$ -edge, with measuring time for 70 min for each sample.

### 3. 結果および考察

Due to the low loading of Ir species in the electrocatalysts, the fluorescence detection mode was carried out to obtain results with high signal to noise ratios. The absorption coefficients ( $\mu(E)$ ) changed with the energy, with the obvious white lines at around 11215 eV (Fig. 1), demonstrating the existence of Ir species in the electrocatalysts (i.e., Ir1 and Ir2). The intensity of the



white line in Ir1 was much higher than that in Ir2, suggesting different oxidation states between the two electrocatalysts<sup>[2]</sup>. Furthermore, Ir1 and Ir2 exhibited distinct fluctuations of  $\mu(E)$  after the absorption edge. Given the scattering effect by the neighboring atoms on the absorption of X-ray at the center Ir atom, those different shapes of  $\mu(E)$  indicated diverse coordination arrangements for the center Ir between Ir1 and Ir2<sup>[3]</sup>. In short, the different electronic and atomic configurations from the XAS results provided important structural information for the two Ir-based electrocatalysts, which contributes to the clarification of the electrocatalytic mechanisms for guiding the optimization of the electrocatalytic materials.

### 4. 参考文献

- 1. Chem. Soc. Rev., 2021, 50, 12897-12914.
- 2. Phys. Chem. Chem. Phys., 2020, 22, 10807-10818.
- 3. Adv. Energy Mater., 2023, 13, 2202913.