

# Identification of Local Structures for Fe Species

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## +-∇-F: Electrocatalyst, Multicomponent materials, Local structure, Fe catalysis

### 1. 背景と研究目的

Fe species play important roles in many electrocatalytic reactions, and the Fe sites usually serve as highly active centres or promoters to significantly enhance the overall electrocatalytic performance<sup>[1]</sup>. However, the clarification of the inner functions of Fe species on electrocatalysis requires a definite exploration on their local structures. In this work, we used a surface-sensitive X-ray adsorption spectroscopy (XAS) method, i.e., conversion electron yield (CEY)-based XAS, to study the electronic structures and atomic configurations of Fe species in our multicomponent electrocatalysts. The disclosed difference in our samples will contribute to the in-depth understanding of the local structure effect of electrode on regulating the electrocatalytic behaviours.

#### 2. 実験内容

The multicomponent electrocatalysts were loaded on metallic substrates. The CEY method was used to collect the XAS of the targeted elements. For each element, it took 2 min to obtain sufficient signals.

#### 3. 結果および考察

The XAS spectra of the two Fe-involved multicomponent electrocatalysts (here we noted as Fe1 and Fe2) were shown in Fig. 1. It is evident that the pre-edge peaks, around 7115 eV, were almost the same in the two samples. This indicated that Fe1 and Fe2 had similar metal-ligand configurations (i.e., the octahedral coordination)<sup>[2]</sup>. However, in the X-ray absorption near edge structure (XANES) region Fe1 and Fe2 showed different fluctuations. This various XANES

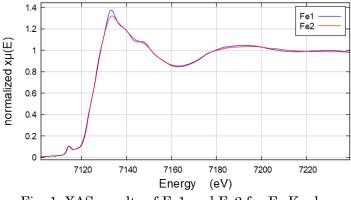


Fig. 1. XAS results of Fe1 and Fe2 for Fe K-edge.

plots suggested that the two Fe species in the samples should have different local atomic structures. This difference may come from the distinct components between Fe1 and Fe2. Further explorations are necessary to reveal more structure details of these samples in the future.

#### 4. 参考文献

- 1. Nature chemistry, 2013, 5(3): 228-233.
- 2. Journal of Synchrotron Radiation, 2015, 22(2): 410-426.