



Observation of Atomically Dispersed Metal Sites Supported on a MOF-Derived Carbon

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Keywords: single-atom catalysts, MOF-derived carbons

1. Background

Single-atom catalysts (SACs), bearing atomically dispersed metal sites, have emerged as a new research field in catalysis. SACs based on two or more different metals have presented better catalytic behaviors compared with their corresponding single metal-based SACs, possibly due to the cooperative effects among different single metal sites. In this experiment, we try to synthesize atomically dispersed Fe, Co, Ni and Zn atoms supported on a single carbon network by pyrolysis of the metal-organic frameworks with loading of corresponding metal species precursors.

2. Experiments

X-ray absorption fine structure (XAFS) analyses of the hierarchically porous carbon networks with Fe, Co, Ni and Zn atoms (FeCoNiZn-NC) were performed at Aichi Synchrotron Radiation Center (BL11S2). Each powder sample pressed as pallets were analyzed.

3. Results and Discussion

Currently, element-selective XAFS, including X-ray absorption near-edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS) spectroscopy, has been considered as a necessary characterization for the MOF-derived single-atom catalysts, which can demonstrate the atomically dispersed metal atoms via verifying the absence of metal-metal bonds in the spectra.¹ So, XAFS analyses were performed to investigate the local environment of single Fe/Co/Ni atoms in FeCoNi-NC. As shown in Figure 1, the obtained Fe/Co/Ni/Zn K-edge XAFS spectra showed that our samples exhibited distinctly different profiles from those of corresponding metal foils (blue lines). The coordination configurations were then determined by the Fourier transformed k^3 -weighted $\chi(k)$ -function of the corresponding EXAFS spectra in R space. We have confirmed the absence of metallic metal-metal coordination in FeCoNiZn-NC, which certified that Fe/Co/Ni/Zn sites should be atomically dispersed in the samples. The on-going data analysis is about the structural fitting by virtue of DFT calculation.

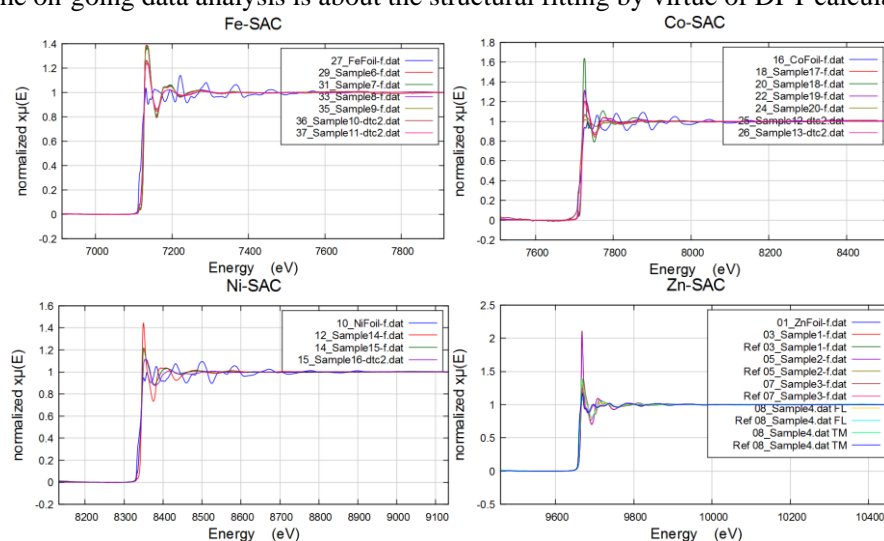


Figure 1. Fe, Co, Ni and Zn K-edge XAFS spectra.

4. Reference

1. Xu, Q. et al. Fabricating Dual-Atom Iron Catalysts for Efficient Oxygen Evolution Reaction: A Heteroatom Modulator Approach. *Angew. Chem., Int. Ed.* 2020, DOI: 10.1002/anie.202007221.