



Observation of Single Fe and Co Atoms Supported on MOF-Derived Carbons

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1. Background

Single-atom catalysts (SACs), with their catalytic sites dispersed at the atomic level, have very recently emerged as a new research frontier in catalysis. Realizing the maximum utilization of active metal sites, SACs usually exhibit ultrahigh activity and even selectivity toward diverse reactions, comparable to their homogeneous counterparts. On the other hand, in comparison with homogeneous metal complexes, SACs present heterogeneous characteristics such as easy separation, excellent reusability, and high stability. Therefore, SACs can serve as an idea bridge that fills the gap between homogeneous and heterogeneous catalysts. In this report, we attempted to synthesize the single-atom catalysts supported on carbon networks by pyrolysis of the metal-organic frameworks.

2. Experiments

XANES and EXAFS analyses of the hierarchically porous carbon networks with Fe and Co atoms (Co/Fe-NC) were performed at Aichi Synchrotron Radiation Center (BL11S2). Each powder sample packed in the plastic tubes were analyzed.

3. Results and Discussion

Currently, XAFS has been considered as a necessary characterization for the MOF-derived single-atom catalysts in the demonstration of atomically dispersed metal atoms via verifying the absence of metal-metal bonds in the spectra.¹ So, XANES and EXAFS analyses were performed to investigate the local environment of single Fe/Co atoms in Co/Fe-NC. In figure 1, the magnitude of Fourier transformed k^2 -weighted Fe/Co K-edge EXAFS spectrum exhibited the main peaks (1–2 Å) could be assigned to the Fe-N and Co-N coordination. The absence of metallic Fe–Fe/Co–Co coordination certified that Fe/Co sites were atomically dispersed in Co/Fe-NC. The on-going data analysis is about the structural fitting by virtue of DFT calculation.

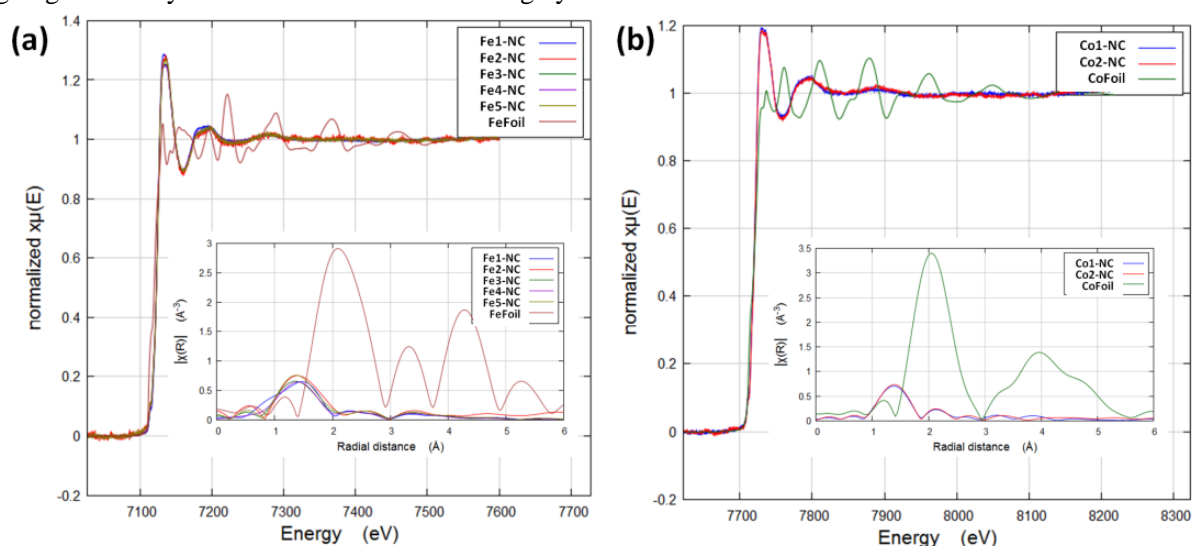


Figure 1. Fe (a) and Co (b) K-edge XANES and their corresponding magnitude of Fourier transformed EXAFS spectra.

4. References

- Xu, Q. et al. Puffing Up Energetic Metal-Organic Frameworks to Large Carbon Networks with Hierarchical Porosity and Atomically Dispersed Metal Sites. *Angew. Chem., Int. Ed.* (2019) 58, 1975-1979.