In-situ XAFS Applications in Energy Materials

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Abstract

In the twenty-first century, the energy shortage and environmental pollution have become two major issues that severely restrict the sustainable development of the world economy, due to the overuse of the fossil energy. One of the most effective strategies to tackle the fossil energy crisis is to develop clean energy conversion processes that can convert molecules in the atmosphere (e.g., water) into higher-value products (e.g., hydrogen). To this end, based on the synchrotron radiation facilities in China, we have developed *in-situ* X-ray absorption fine structure (XAFS) spectroscopies and performed systematic investigations on the energy conversion mechanisms over a series of advanced energy-related low-dimensional materials.

By using the *in-situ* XAFS technique, we report the atomic-level identification of a high-valence $HO\text{-}Co_1\text{-}N_2$, near-free Pt single site, or NiFe-MOF moiety during the catalytic water splitting processes, and further unravel the preferred water adsorption reaction intermediates on a single-atom or low-dimensional catalyst [1-4]. For the electrochemical water splitting, Our XAFS characterization results clarified that the unique surface defects and disordered structure in the low-dimensional materials can increase the electron density and then enhance the electrocatalytic activity [5-7]. Whereas for the photocatalytic water splitting, Our XAFS characterization results demonstrated that the unique band structures of the low-dimensional materials can regulate the photoexcited carriers transfer and then improve the quantum efficiency of the solar energy conversion [8-10]. All these results can help to guide the design and synthesis of high-performance and low-cost energy conversion materials.

References

1. L.L. Cao, T. Yao, S.Q. Wei, et al. *Nature Catalysis* 2, 134 (2019).
2. W.R. Cheng, Q.H. Liu, et al. *Nature Energy* 4, 115 (2019).
3. H. Su, W.R. Cheng, Q.H. Liu et al. *J. Am. Chem. Soc.* 142, 12306 (2020).
4. H. Su, W.R. Cheng, Q.H. Liu et al. *ACS Energy Lett.* 142, 12306 (2020).
5. W. Liu, Q.H. Liu, T. Yao, S.Q. Wei, et al. *Angew. Chem. Int. Ed.* 56, 9312 (2017).
6. J.H. Huang, Q.H. Liu, S.Q. Wei, et al. *Angew. Chem. Int. Ed.* 54, 8722 (2015).
7. Y.Y. Huang, W.R. Cheng, Q.H. Liu, et al. *J. Mater. Chem. A* 6, 3202 (2018).
8. J.H. Huang, Q.H. Liu, S.Q. Wei, et al. *Angew. Chem. Int. Ed.* 55, 2137 (2016).
9. Q. H. Liu, Y. Xie, Z.Y. Wu, S.Q. Wei, et al. *Nature Commun.* 5, 5122 (2014).
10. W. Che, Q.H. Liu, S.Q. Wei, et al. *J. Am. Chem. Soc.* 139, 3021 (2017).

Biography

Dr. Qinghua Liu is currently a professor of National Synchrotron Radiation Laboratory, University of Science and Technology of China (USTC). He received his Ph.D. in 2009 from USTC, and then did research work on renewable energy conversion and synchrotron radiation experimental techniques. His current research interests focus on the synthesis and characterizations of advanced energy functional nanomaterials for photocatalytic, electrochemical, and photoelectrochemical applications and the development of advanced in situ/operando synchrotron radiation experimental techniques and their applications in energy storage and reaction mechanism.

The specific research fields and achievements of Dr. Qinghua Liu are as follows,

(1) Development of *in-situ/operando* X-ray absorption spectroscopy methods

Developing *in-situ/operando* X-ray absorption spectroscopy (XAFS) and infrared (IR) spectroscopy methods in order to investigate the energy conversion mechanics at the solid-liquid interface of the advanced low-dimensional energy conversion materials.

(2) Design of advanced low-dimensional energy conversion materials

Designed a series of advanced low-dimensional energy conversion materials, such as NiFe-MOFs, Co-NC, Ni-NC, Au_1N_x, CoOOH, and TiO_2 based single atom, one-dimensional nanotube and/or two-dimensional nanosheet materials and greatly improved the energy conversion efficiency.

(3) Investigation on the energy conversion mechanisms of energy materials

Using the developed *in-situ/operando* synchrotron characterization methods to investigate the energy conversion mechanics of the advanced energy materials.