Title: XAFS in Energy Materials

Tao Yao, Shiqiang Wei
yaot@ustc.edu.cn
National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230029, P. R. China

In the twenty-first century, with a rising global population, increasing energy demands, and impending climate change, a blossoming interest have been raised over the security of our energy future. One of the most effective strategies to tackle the fossil energy crisis is to develop photoelectrochemical conversion processes that can convert molecules in the atmosphere (e.g., water, carbon dioxide, and nitrogen) into higher-value products (e.g., hydrogen, hydrocarbons, and ammonia) by coupling to renewable energy. To this end, based on the synchrotron radiation X-ray absorption fine structure (XAFS) spectroscopy, we have performed systematic investigations on the structure and performance of energy-related low-dimensional materials.

We have designed a series of novel atomically dispersed single-site and atomically thick two-dimensional materials, which exhibited high performance in energy conversion reactions (e.g. photo/electrochemical water splitting, photo/electrochemical CO_2 reduction). By using XAFS as a powerful characterization technique, we report an atomic-level insight, design, and fabrication of single Co site grafted on g-C_3N_4 nanosheets as a prototypical photocatalyst for efficient H_2 production [1,2]. This coordinatively unsaturated single Co site can effectively suppress charge recombination and prolong carrier lifetime. As a result, the composite single-site photocatalyst exhibits steady and high hydrogen production and quantum efficiency. Meanwhile, we have clarified that the unique surface defects and disordered structure in the two-dimensional ultrathin materials can increase the electron density and enhance the charge separation and transportation, thus enhancing the efficiency of solar energy conversion [3]. Regarding to the electrocatalytic water splitting and carbon dioxide reduction, by using XAFS spectroscopy, we have unveiled the atomic and electronic structures, such as coordination number, structural defects and disorder, and chemical states, of surface active sites of low-dimensional electrocatalysts. Combining the first-principle calculations, we correlated the structures of active site to the reduction of overpotential for the electrocatalytic hydrogen or oxygen evolution in water splitting, as well as the lowered of activation energy for carbon dioxide electroreduction [4,5]. Moreover, we have developed synchrotron radiation in-situ X-ray spectroscopy for the operando investigations of energy materials under photo-/electro-catalytic reactions. The above results can help to guide the design and synthesis of high-performance and low-cost energy conversion materials.

References:

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