In situ formic acid dehydrogenation observation using a UV-vis-diffuse-reflectance

spectroscopy system

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In recent decades, formic acid (FA) is regarded as one of the most promising liquid hydrogen carriers, which possesses a high hydrogen content (53 g of H_2/L) and is nontoxic, and has garnered considerable attention.

With regard to formic acid dehydrogenation (FADH), researchers have mainly focused on the development of efficient catalysts; thus, a myriad of homogeneous catalysts have been developed so far¹⁻³. However, few in situ measurements have been reported during the gas generation to understand the FADH reaction mechanism in the presence of homogeneous catalysts. One of the barriers to employing conventional in situ measurements of the absorption spectra is the presence of gas-liquid mixed phases. Herein, we developed a new in situ UV-vis-diffuse-reflectance spectroscopy technology to monitor the



Fig.1 The absorption spectra of the sample

Fig.2 The absorption spectra of long-term experiments

FADH reaction. The results (Figure 1) showed a clear signal at 215 nm corresponding to the FA in the sample and the weak signals of the catalyst (Ir-4DHBP) were obtained as well. Moreover, we applied our new technology to monitor the sample in the long-term experiment (> 14h), and it was found that the peak of the FA decreased gradually which indicated the consumption of the FA and a new signal appeared in the range from 650 to 700 nm which probably corresponds to the intermediate in the process of the catalyst decomposition. In this presentation, we will introduce the detail in the mechanism of the catalyst decomposition investigated by our new technology.

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