Application of XAS to studies of single atom catalysis and design of EXAFS catalysis reactor

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Studies of single site catalysts have attracted significant efforts in the community of catalysis due to the distinct catalytic behavior of this type of catalysts. This distinction origins at different coordination environment of the singly dispersed catalyst atoms in contrast to the continuously packed metal or cationic sites. XAS (XANES and EXAFS) is important technique in identifying chemical and coordinating environment of interested atoms. With feature of working in gas phase due to its photo-in-photo-out nature, XAS has been the main technique in studying the chemical and structural natures of single site catalysts. In the last a few years, we have used this technique in identifying structural environments of catalyst atoms of single atom catalysts in ex situ, in situ or under operando catalytic condition. Through correlating with catalytic performance, we have also established correlations between catalyst structure and the corresponding catalytic performance. Through this correlation, we achieved fundamental understanding of catalysis at a molecular level. In this talk, I will present examples for single site catalysts in gas phase and liquid phase including the transformation of methane to methanol and acetic acid on singly dispersed Rh atoms anchored in zeolite liquid and partial oxidation of methane to syngas on single Rh atoms anchored on transition metal oxides. Other than the structural characterization and catalytic performance, I will present design of three different EXAFS reactors we built for tracking chemical and coordination environments of catalyst in a gas phase at high pressure or in liquid phase under a gas phase at high reactants.

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